

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: TRUBS, Wc Examiner #: 69332 Date: 3/14/05
Art Unit: 1711 Phone Number 302-1281 Serial Number: 12728588
Mail Box and Bldg/Room Location: 12571 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: _____

Inventors (please provide full names): _____

Earliest Priority Filing Date: _____

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

General formula (i) of claim 1 derived from
formula (c) in the presence of an acid catalyst in
claims 3-5. Ethers

SCIENTIFIC REFERENCE B:
Sci & Tech Inf. Ctr

MAR 14 RECD

Pat. & T.M. Office

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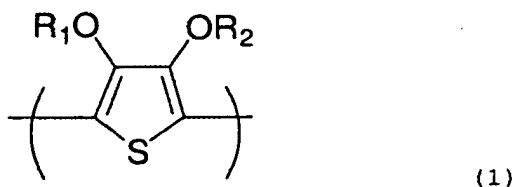
	Type of Search	Vendors and cost where applicable
Searcher: <u>EL</u>	NA Sequence (#) _____	STN _____
Searcher Phone #: _____	AA Sequence (#) _____	Dialog _____
Searcher Location: _____	Structure (#) _____	Questel/Orbit _____
Date Searcher Picked Up: _____	Bibliographic _____	Dr. Link _____
Date Completed: <u>3-22-05</u>	Litigation _____	Lexis/Nexis _____
Searcher Prep & Review Time: _____	Fulltext _____	Sequence Systems _____
Clerical Prep Time: _____	Patent Family _____	WWW/Internet _____
Online Time: _____	Other _____	Other (specify) _____

6/728,088

WHAT IS CLAIMED IS:

1. A process for preparing conductive polythiophenes comprised of structural units of the general formula (1):

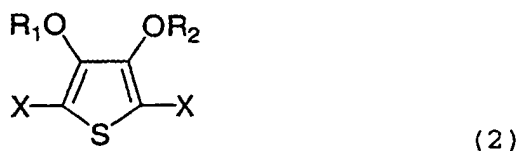
5



where R_1 and R_2 independently represent hydrogen or a C_1 - C_4 alkyl group, or together represent an optionally substituted C_1 - C_4 alkylene group, preferably an optionally alkyl-substituted methylene group, an optionally C_1 - C_4 alky- or phenyl-substituted 1,2-ethylene group, a 1,3-propylene group or a 1,2-cyclohexylene group;

which are prepared from 2,5-dihalothiophene of the general formula (2):

15



where R_1 and R_2 are described as above in the general formula (1), and X is a halogen atom selected from Cl, Br and I;

20 in the presence of an acid catalyst.

2. A process for preparing polythiophenes according to claim 1, wherein R_1 and R_2 independently represent methylene, 1,2-ethylene or 1,3-propylene.

5 3. A process for preparing polythiophene according to claim 1 or 2, wherein the acid catalyst is a Lewis acid, protic acid, organic acid or polymeric acid.

4. A process for preparing polythiophenes according to claim 3, wherein the Lewis acid catalyst is a boron salt, zinc salt, tin salt or iron salt; the protic acid catalyst is phosphoric acid, sulfuric acid, nitric acid, hypochlorous acid, HF, HCl, HBr or HI; the organic acid catalyst is carboxylic acid or sulfonic acid; polymeric acid catalyst is 15 polystyrenesulfonic acid, polyacrylic acid, polymethacrylic acid, polymaleic acid or polyvinylsulfonic acid; and the catalyst is used individually or as a mixture of two or more.

5. A process for preparing polythiophenes according to claim 4, wherein the boron salt is boron trifluoride, boron 20 trifluoride dihydrate, boron trifluoride diethyl etherate, boron trifluoride-alcohol complex, boron trifluoride-methyl sulfide complex, boron trifluoride-phosphoric acid complex, boron trichloride, boron trichloride-methyl sulfide complex, 25 boron tribromide, or boron tribromide-methyl sulfide complex,

used individually or as a mixture of two or more.

6. A process for preparing polythiophenes according to any one of claims 1 to 5, wherein the solvent is a C₆-C₂₀ aliphatic or aromatic hydrocarbon, halogen-containing hydrocarbon, ketone, ether, C₂-C₂₀ alcohol, sulfoxide, amide and water, or a mixture thereof.

7. A process for preparing polythiophene according to claim 6, where the solvent is a C₆-C₂₀ aliphatic or aromatic hydrocarbon including alkanes, alkylbenzenes and phenol; halogen-containing hydrocarbon including alkanes and halobenzenes containing halogen substituent(s); ketone including acetone, propanone, butanone, pentanone, hexanone, heptanone, octanone and acetophenone; ether including diethyl ether, tetrahydrofuran (THF), dipropyl ether, dibutyl ether, methyl butyl ether, diphenyl ether, dioxane, diglyme, diethylene glycol and ethylene glycol (EG); sulfoxide including dimethylsulfoxide (DMSO); amide including N,N-dimethylformamide (DMF), N-methylacetamide (NMAA), N,N-dimethylacetamide (DMA), N-methylpropionamide (NMPA) and N-methylpyrrolidinone (NMP), used either individually or as a mixture of two or more.

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FILE 'LREGISTRY'

L1 STR
L2 STR L1

FILE 'REGISTRY'

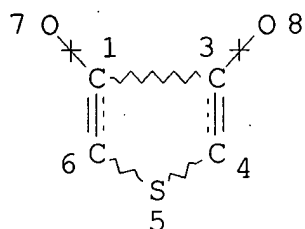
L3 2 S L1
L4 SCR 2043 OR 1976
L5 10 S L1 AND L4
L6 633 S L1 AND L4 FUL
SAV L6 TRU088/A
L7 483 S L6 AND PMS/CI
L8 227 S L6 AND 1<X
L9 77 S L7 AND L8
L10 6 S L2 SSS SAM SUB=L6
L11 48 S L2 SSS FUL SUB=L6
SAV L11 TRU088A/A
L12 26 S L11 AND L7
L13 22 S L11 NOT L12
L14 457 S L7 NOT L12

FILE 'HCA'

L15 29 S L12
L16 30 S L13
L17 2609 S L14
L18 15 S L16 AND L17
L19 4 S L15 AND ACID?
L20 4 S L16 AND ACID?
L21 44383 S LEWIS#
L22 10868 S BRONSTED# OR BROENSTED#
L23 1 S L15 AND (L21 OR L22)
L24 0 S L16 AND (L21 OR L22)
L25 6 S L19 OR L20 OR L23
L26 29 S (L15 OR L18) NOT L25
L27 26 S L16 NOT L25
L28 4 S L16 NOT (L26 OR L27)

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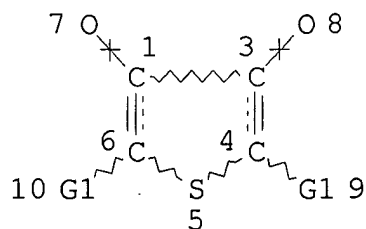
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L1 STR



NODE ATTRIBUTES:
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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 7

STEREO ATTRIBUTES: NONE
L2 STR



VAR G1=CL/BR/I
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE
L4 SCR 2043 OR 1976
L6 633 SEA FILE=REGISTRY SSS FUL L1 AND L4
L11 48 SEA FILE=REGISTRY SUB=L6 SSS FUL L2

100.0% PROCESSED 65 ITERATIONS

48 ANSWERS

SEARCH TIME: 00.00.01

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FILE 'HCA'

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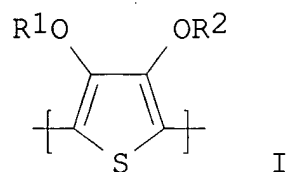
=> d 125 1-6 cbib abs hitstr it

L25 ANSWER 1 OF 6 HCA COPYRIGHT 2005 ACS on STN

141:226365 Processes for preparing conductive macromolecular polythiophenes using **acid** catalysts. Baik, Woon-phil; Kim, Young-sam; Park, Jae-han; Jung, Sang-gook (Myongji University, S. Korea). U.S. Pat. Appl. Publ. US 2004171790 A1 20040902, 5 pp. (English). CODEN: USXXCO. APPLICATION: US 2003-728088 20031205. PRIORITY: KR 2002-77465 20021206.

Significant

GI



AB The polythiophene I (R1, R2 = H, (un)substituted C1-4 alkyl, (un)substituted 1,2-ethylene, 1,3-propylene or 1,2-cyclohexylene group) is prepd. by cationic polymn. from 2,5-dihalo thiophene in the presence of an **acid** catalyst, such as **Lewis acid**, **protic acid**, **oxygen acid**, or **polymeric acid**. The cond. of the resulting polythiophene is 255 S/cm under optimal conditions. Thus, 20.0 g 2,5-dibromo-3,4-ethylenedioxythiophene was mixed with toluene 400 and boron trifluoride 26 mL at room temp. for 4 h and heated to 100° for 24 h to give 12.9 g poly(3,4-ethylenedioxythiophene) which having cond. 255 S/cm.

IT 350037-71-7P 748185-34-4P 748185-35-5P

(processes for prepg. conductive macromol. polythiophenes using **acid** catalysts)

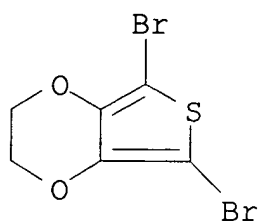
RN 350037-71-7 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 174508-31-7

CMF C6 H4 Br2 O2 S



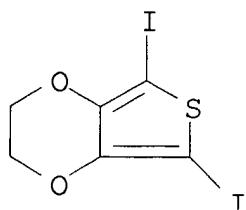
RN 748185-34-4 HCA

CN Thieno[3,4-b]-1,4-dioxin, 2,3-dihydro-5,7-diiodo-, homopolymer (9CI)
(CA INDEX NAME)

CM 1

CRN 640737-72-0

CMF C6 H4 I2 O2 S



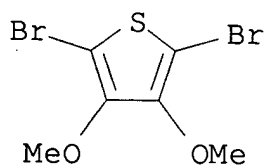
RN 748185-35-5 HCA

CN Thiophene, 2,5-dibromo-3,4-dimethoxy-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 345666-04-8

CMF C6 H6 Br2 O2 S



- IT Polymerization catalysts
(cationic; processes for prepg. conductive macromol. polythiophenes using **acid** catalysts)
- IT **Acids**, uses
(org.; processes for prepg. conductive macromol. polythiophenes using **acid** catalysts)
- IT **Acids**, uses
Carboxylic **acids**, uses
Lewis **acids**
Sulfonic **acids**, uses
(processes for prepg. conductive macromol. polythiophenes using **acid** catalysts)
- IT 109-63-7, Boron trifluoride diethyl etherate 353-43-5 1428-24-6, Boron trifluoride-triphenyl phosphate complex (1:1) 5523-19-3, Boron trichloride-dimethyl sulfide (1:1) 7439-89-6D, Iron, salts 7440-31-5D, Tin, salts 7440-42-8D, Boron, salts 7440-66-6D, Zinc, salts 7637-07-2, Boron trifluoride, uses 7646-85-7, Zinc chloride, uses 7647-01-0, Hydrochloric **acid**, uses 7664-38-2, Phosphoric **acid**, uses 7664-39-3, Hydrofluoric **acid**, uses 7664-93-9, Sulfuric **acid**, uses 7697-37-2, Nitric **acid**, uses 7790-92-3, Hypochlorous **acid** 9003-01-4, Polyacrylic **acid** 10034-85-2, Hydroiodic **acid** 10035-10-6, Hydrobromic **acid**, uses 10294-33-4, Boron tribromide 10294-34-5, Boron trichloride 13319-75-0, Boron trifluoride dihydrate 25087-26-7, Polymethacrylic **acid** 26099-09-2, Polymaleic **acid** 26101-52-0, Polyvinylsulfonic **acid** 29957-59-3 50851-57-5, Polystyrenesulfonic **acid**
(processes for prepg. conductive macromol. polythiophenes using **acid** catalysts)
- IT 120326-42-3P, Poly(3,5-dimethoxy-2,5-thiophenediyl)
350037-71-7P 748185-34-4P 748185-35-5P
(processes for prepg. conductive macromol. polythiophenes using **acid** catalysts)
- L25 ANSWER 2 OF 6 HCA COPYRIGHT 2005 ACS on STN
- 139:93393 Characterization of Organic p/n Junction Photodiodes Based on Poly(alkylthiophene)/Perylene Diimide Bilayers. Tan, Li; Curtis, M. David; Francis, A. H. (Macromolecular Science & Engineering Center and Department of Chemistry, The University of Michigan, Ann Arbor, MI, 48109-1055, USA). Chemistry of Materials, 15(11), 2272-2279 (English) 2003. CODEN: CMATEX. ISSN: 0897-4756. Publisher: American Chemical Society.
- AB Photoconduction of bilayer org. p/n junction photocells can be finely tuned through the alteration of either the side chain orientation (regiorandom vs. regioregular) or main chain structure in poly(3-alkylthiophene)s (P3ATs), where the incorporation of an electron-donating group (EDOT) appears to be an excellent method for

enhancing the photoconduction. also, doping of P3ATs proved to be an equally viable route for tuning the device characteristics. These polymers were used to fabricate bilayer org. photocells with the polymer as the p-type layer and 1,2-diaminobenzeneperylene-3,4,9,10-tetracarboxylic acid diimide (PV) as the n-type layer.

Action spectra at steady-state illumination demonstrated that all the interfaces (org.-org. p/n junction and org.-electrode) are actively involved in the photogeneration of carriers. Crit. device properties, for example, open-circuit voltage (Voc) and short-circuit current (Isc), are not only dependent on the selection of electrodes and org. materials but also greatly affected by the illumination wavelength and intensity.

IT 554459-31-3P, 2,5-Dibromo-3-butylthiophene-2,5-dibromo-3,4-ethylenedioxythiophene copolymer
(prepn. and properties of)

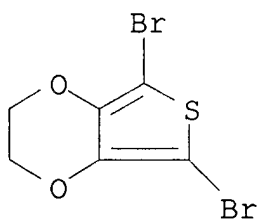
RN 554459-31-3 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro-, polymer with 2,5-dibromo-3-butylthiophene (9CI) (CA INDEX NAME)

CM 1

CRN 174508-31-7

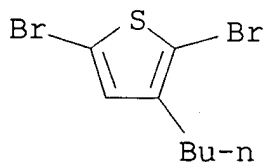
CMF C6 H4 Br2 O2 S



CM 2

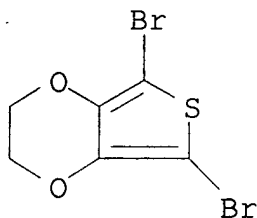
CRN 116971-10-9

CMF C8 H10 Br2 S



IT 174508-31-7P, 2,5-Dibromo-3,4-ethylenedioxythiophene
(prepn. of)

RN 174508-31-7 HCA
CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro- (9CI) (CA INDEX NAME)

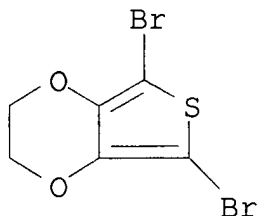


- IT Electric current carriers
(generation; properties of org. pn photodiodes based on polyalkylthiophenes and diaminobenzeneperylenetetracarboxylic **acid diimide**)
- IT Glass substrates
(in fabrication of org. pn photodiodes based on polyalkylthiophenes and diaminobenzeneperylenetetracarboxylic **acid diimide**)
- IT Cyclic voltammetry
(of polyalkylthiophene derivs.)
- IT Band gap
(optical; of polyalkylthiophene derivs.)
- IT Conducting polymers
(polythiophenes; properties of org. pn photodiodes based on polyalkylthiophenes and diaminobenzeneperylenetetracarboxylic **acid diimide**)
- IT Absorption spectra
Dopants
Electric current-potential relationship
Electrodes
Open circuit potential
Optical absorption
Photoconductivity
Photocurrent
Photodiodes
Short circuits
Solid-solid interface
(properties of org. pn photodiodes based on polyalkylthiophenes and diaminobenzeneperylenetetracarboxylic **acid diimide**)
- IT Coating process
(spin; in fabrication of org. pn photodiodes based on polyalkylthiophenes and diaminobenzeneperylenetetracarboxylic **acid diimide**)
- IT 104-15-4, Toluenesulfonic **acid**, uses 7647-01-0, Hydrogen chloride, uses 7664-93-9, Sulfuric **acid**, uses

- 14635-75-7, Nitrosonium tetrafluoroborate
(P3OT dopant; properties of org. pn photodiodes based on polyalkylthiophenes and diaminobenzeneperylenetetracarboxylic acid diimide)
- IT 98837-51-5, Poly(3-butylthiophene)
(UV spectra of)
- IT 7440-22-4, Silver, uses
(contact; properties of org. pn photodiodes based on polyalkylthiophenes and diaminobenzeneperylenetetracarboxylic acid diimide)
- IT 116971-10-9, 2,5-Dibromo-3-butylthiophene
(in prepn. of butylthiophene-ethylenedioxythiophene copolymer)
- IT 126213-50-1, 3,4-Ethylenedioxythiophene
(in prepn. of dibromoethylenedioxythiophene)
- IT 554459-31-3P, 2,5-Dibromo-3-butylthiophene-2,5-dibromo-3,4-ethylenedioxythiophene copolymer
(prepn. and properties of)
- IT 174508-31-7P, 2,5-Dibromo-3,4-ethylenedioxythiophene
(prepn. of)
- IT 50926-11-9, ITO 55034-79-2
(properties of org. pn photodiodes based on polyalkylthiophenes and diaminobenzeneperylenetetracarboxylic acid diimide)
- IT 104934-51-2, Poly(3-octylthiophene)
(pure and doped; properties of org. pn photodiodes based on polyalkylthiophenes and diaminobenzeneperylenetetracarboxylic acid diimide)
- IT 7664-41-7, Ammonia, processes
(redn. of doped P3OT with; properties of org. pn photodiodes based on polyalkylthiophenes and diaminobenzeneperylenetetracarboxylic acid diimide)
- L25 ANSWER 3 OF 6 HCA COPYRIGHT 2005 ACS on STN
- 137:232315 Optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers. Apperloo, Joke J.; Groenendaal, L. "Bert"; Verheyen, Hilde; Jayakannan, Manickam; Janssen, Rene A. J.; Dkhissi, Ahmed; Beljonne, David; Lazzaroni, Roberto; Bredas, Jean-Luc (Laboratory for Macromolecular and Organic Chemistry, Eindhoven University of Technology, Eindhoven, 5600 MB, Neth.). Chemistry--A European Journal, 8(10), 2384-2396 (English) 2002. CODEN: CEUJED. ISSN: 0947-6539. OTHER SOURCES: CASREACT 137:232315. Publisher: Wiley-VCH Verlag GmbH.
- AB The optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers (EDOT_n, n = 1-4) and their β,β' -unsubstituted analogs (T_n, n = 1-4) are described. Both series are end capped with Ph groups to prevent irreversible α -coupling reactions during oxidative doping. Absorption and fluorescence spectra of both series reveal a significantly higher degree of intrachain conformational order in the EDOT_n oligomers.

Oxidn. potentials (EPA1 and EPA2) detd. by cyclic voltammetry reveal that those of EDOTn are significantly lower than the corresponding Tn oligomers as a consequence of the electron-donating 3,4-ethylenedioxy substitution. Linear fits of EPA1 and EPA2 vs. the reciprocal no. of double bonds reveal significantly steeper slopes for the EDOTn than for the Tn oligomers. This could indicate a more effective conjugation for the EDOTn series, confirmed by the fact that coalescence of EPA1 and EPA2 is reached already at relatively short chain lengths (≈ 5 EDOT units) in contrast to the Tn series (> 10 thiophene units). The stepwise chem. oxidn. of the EDOTn and Tn oligomers in soln. was carried out to obtain radical cations and dications. The energies of the optical transitions of the radical cations and dications as detd. by UV/Vis/NIR spectroscopy were similar for the two series. These spectroscopic observations are consistent with quantum-chem. calcns. performed on the singly charged mols. Cooling solns. contg. $T2^{\bullet+}$, $T3^{\bullet+}$, $EDOT2^{\bullet+}$, and $EDOT3^{\bullet+}$ revealed the reversible formation of dimers, albeit with a some-what different tendency, expressed in the values for the dimerization enthalpy.

IT **174508-31-7P**, 2,5-Dibromo-3,4-ethylenedioxythiophene
 (coupling; prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
 RN 174508-31-7 HCA
 CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro- (9CI) (CA INDEX NAME)



IT Radical ions
 (cations, formation, electronic and ESR spectra, and dimerization; prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
 IT Exciton
 (coupling in radical cation dimers; prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
 IT Cations
 (divalent; prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
 IT Substituent effects
 (ethylenedioxy; prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)

- IT CI (molecular orbital method)
Oscillator strength
(in electronic excitation of radical cations; prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
- IT Conformation
(intrachain conformational order; prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
- IT Dimerization
Dimerization enthalpy
ESR (electron spin resonance)
Electronic excitation
Hyperfine coupling
(of radical cations; prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
- IT Chemical chains
Fluorescence
Homologous series
Oxidation potential
UV and visible spectra
Vibronic excitation
(prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
- IT Oligomers
(prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
- IT Conjugation (bond)
(π -; prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
- IT 29488-24-2, 2-Bromo-5-phenylthiophene
(boronation; prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
- IT 591-50-4, Iodobenzene 625-88-7, 2,5-Diiodothiophene 3339-80-8,
5,5'-Diiodo-2,2'-bithiophene 24388-23-6 104499-99-2,
5,5''-Diiodo-2,2':5',2''-terthiophene 264282-36-2
(coupling; prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
- IT **174508-31-7P**, 2,5-Dibromo-3,4-ethylenedioxythiophene
459409-70-2P 459409-71-3P 459409-73-5P 459409-74-6P
(coupling; prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
- IT 76-09-5, Pinacol
(cyclocondensation with boronic acid; prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
- IT 205436-42-6 459409-82-6
(dimerization; prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)

- IT 1665-32-3P, 5,5''-Diphenyl-2,2':5',2''-terthiophene 83495-30-1P,
5,5'-Diphenyl-2,2'-bithiophene 459409-75-7P 459409-76-8P
459409-77-9P
(electro- and chem. oxidn.; prepn. and optical and redox
properties of a series of 3,4-ethylenedioxythiophene oligomers)
- IT 238397-97-2P, 5,5'''-Diphenyl-2,2':5',2'':5'',2'''-quaterthiophene
(electro- and chem. oxidn.; prepn. and optical and redox
properties of a series of 3,4-ethylenedioxythiophene oligomers)
- IT 1445-78-9P, 2,5-Diphenylthiophene 459409-78-0P
(electrooxidn.; prepn. and optical and redox properties of a
series of 3,4-ethylenedioxythiophene oligomers)
- IT 185258-96-2 459409-83-7
(oxidn. and dimerization; prepn. and optical and redox properties
of a series of 3,4-ethylenedioxythiophene oligomers)
- IT 459409-85-9
(oxidn.; prepn. and optical and redox properties of a series of
3,4-ethylenedioxythiophene oligomers)
- IT 459409-79-1P 459409-80-4P
(prepn. and optical and redox properties of a series of
3,4-ethylenedioxythiophene oligomers)
- IT 459409-81-5 459409-84-8 459409-86-0 459409-87-1 459409-88-2
(prepn. and optical and redox properties of a series of
3,4-ethylenedioxythiophene oligomers)
- IT 98-80-6, Phenylboronic acid
(prepn. and optical and redox properties of a series of
3,4-ethylenedioxythiophene oligomers)
- IT 126213-50-1, 3,4-Ethylenedioxythiophene
(reactions; prepn. and optical and redox properties of a series
of 3,4-ethylenedioxythiophene oligomers)
- IT 459409-72-4P
(reactions; prepn. and optical and redox properties of a series
of 3,4-ethylenedioxythiophene oligomers)
- IT 195602-17-6
(stannylation; prepn. and optical and redox properties of a
series of 3,4-ethylenedioxythiophene oligomers)

L25 ANSWER 4 OF 6 HCA COPYRIGHT 2005 ACS on STN

136:279781 Electrochemical, conductive, and magnetic properties of
2,7-carbazole-based conjugated polymers. Zotti, Gianni; Schiavon,
Gilberto; Zecchin, Sandro; Morin, Jean-Francois; Leclerc, Mario
(Istituto di Polarografia ed Elettrochimica Preparativa, Consiglio
Nazionale delle Ricerche, Padua, 35020, Italy). Macromolecules,
35(6), 2122-2128 (English) 2002. CODEN: MAMOBX. ISSN: 0024-9297.
Publisher: American Chemical Society.

AB Novel poly(2,7-carbazole)s (i.e., poly(N-octyl-2,7-carbazole-diyl)
and poly(N-(4-hexyl-benzoyl)-2,7-carbazole-diyl)) and their
alternating thiophene, bi-thiophene, and 3,4-ethylenedioxy-2,5-
thienylene copolymers have been investigated by cyclic voltammetry,

UV-vis spectroelectrochem., electrochem. quartz crystal microbalance, in-situ ESR, and in-situ cond. techniques. All polymer films undergo reversible oxidn. and partially reversible redn. processes. In poly(N-octyl-2,7-carbazole-diyl), two isoelectronic oxidn. processes produce radical cations and dication with charge localization at the carbazole subunits. The presence of a strong electron-withdrawing substituent onto the nitrogen atom in the homopolymer leads to an increase by 3 orders of magnitude of the cond. (i.e., $1 + 10^{-2}$ S/cm). Similarly, in alternating copolymers, the oxidative charge is more delocalized over the polyconjugated backbone with in-situ conductivities in the range of $4 + 10^{-2}$ to 10^{-3} S/cm.

IT 406726-97-4P

(2,7-carbazole-based conjugated polymers)

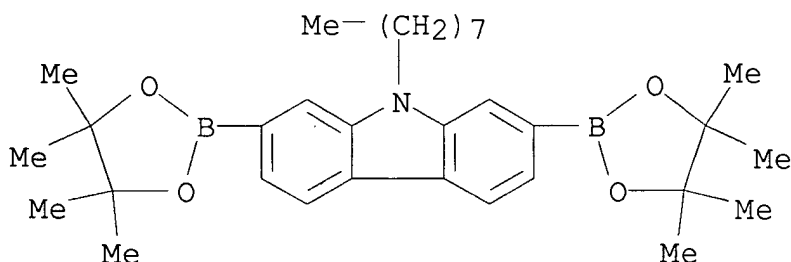
RN 406726-97-4 HCA

CN 9H-Carbazole, 9-octyl-2,7-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-, polymer with 5,7-dibromo-2,3-dihydrothieno[3,4-b]-1,4-dioxin (9CI) (CA INDEX NAME)

CM 1

CRN 406726-92-9

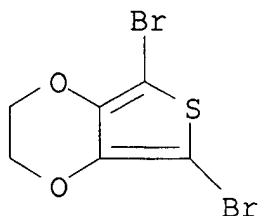
CMF C32 H47 B2 N O4



CM 2

CRN 174508-31-7

CMF C6 H4 Br2 O2 S



- IT Cyclic voltammetry
 - ESR (electron spin resonance)
 - Optical absorption
 - Oxidation
 - Oxidation potential
 - Polymerization catalysts
 - Redox potential
 - (2,7-carbazole-based conjugated polymers)
- IT Polymers, preparation
 - (conjugated, carbazole group-contg.; 2,7-carbazole-based conjugated polymers)
- IT Band gap
- Electric conductivity
 - (electrochem. and optical; 2,7-carbazole-based conjugated polymers)
- IT Conducting polymers
 - (polythiophenes, carbazole group-contg.; 2,7-carbazole-based conjugated polymers)
- IT 75-05-8, Acetonitrile, uses
 - (2,7-carbazole-based conjugated polymers)
- IT 406726-95-2P 406726-96-3P **406726-97-4P** 406726-98-5P
 406726-99-6P 406727-00-2P 406727-01-3P 406727-02-4P
 (2,7-carbazole-based conjugated polymers)
- IT 111-83-1, 1-Bromooctane 358-23-6, Trifluoromethanesulfonic anhydride 5344-78-5, 4-Bromo-3-nitroanisole 5720-07-0, 4-Methoxyphenylboronic **acid** 25015-63-8, Pinacolborane 115297-58-0
 (2,7-carbazole-based conjugated polymers)
- IT 13606-06-9P, 4,4'-Dimethoxy-2-nitro-1,1'-biphenyl 61822-18-2P, 2,7-Dimethoxycarbazole 406726-86-1P 406726-87-2P 406726-88-3P 406726-89-4P
 (2,7-carbazole-based conjugated polymers)
- IT 50606-95-6, 4-Hexylbenzoyl chloride 102871-58-9, 2,7-Dichlorocarbazole
 (monomer synthesis; 2,7-carbazole-based conjugated polymers)
- IT 406726-90-7P 406726-91-8P 406726-92-9P 406726-93-0P
 (monomer; 2,7-carbazole-based conjugated polymers)
- IT 603-35-0, Triphenylphosphine, uses 7447-41-8, Lithium chloride, uses 13965-03-2, Bis(triphenylphosphine)palladium dichloride 14221-01-3, Tetrakis(triphenylphosphine)palladium
 (polymn. catalyst; 2,7-carbazole-based conjugated polymers)

L25 ANSWER 5 OF 6 HCA COPYRIGHT 2005 ACS on STN

131:5811 Temperature-dependent electrical conductivity of p-doped poly(3,4-ethylenedioxythiophene) and poly(3-alkylthiophene)s. Yamamoto, Takakazu; Abila, Mahmut; Shimizu, Takahisa; Komarudin, Dahrma; Lee, Bang-Lin; Kurokawa, Eriko (Research Laboratory

Resources Utilization, Tokyo Institute Technology, Yokohama, 226, Japan). Polymer Bulletin (Berlin), 42(3), 321-327 (English) 1999. CODEN: POBUDR. ISSN: 0170-0839. Publisher: Springer-Verlag.

AB Temp.-dependent elec. cond. of the substituted polythiophenes poly(3,4-ethylenedioxythiophene) (PEDOTh) and head-to-tail type poly(3-alkylthiophene) (HT-P3RTh) was measured. The elec. cond. (σ) of p-doped PEDOTh and HT-P3RTh obeys equations of a type, $\ln \sigma = \ln \sigma_0 - (T_0/T)^{0.25}$, with the T_0 value of ≈ 105 - 107 K.

IT 225518-50-3P
(iodine- and iron tetrachloride-doped; temp.-dependent elec. cond. of p-doped substituted polythiophenes)

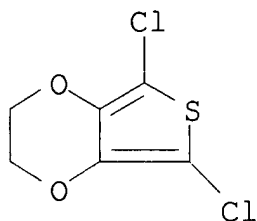
RN 225518-50-3 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dichloro-2,3-dihydro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 225518-49-0

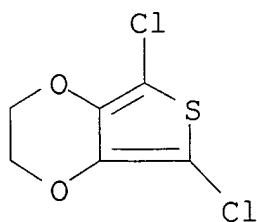
CMF C6 H4 Cl2 O2 S



IT 225518-49-0P
(monomer; temp.-dependent elec. cond. of p-doped substituted polythiophenes)

RN 225518-49-0 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dichloro-2,3-dihydro- (9CI) (CA INDEX NAME)



IT Polymers, properties
(polythiophenes; temp.-dependent elec. cond. of p-doped

- substituted polythiophenes)
- IT Conducting polymers
Electric conductivity
(temp.-dependent elec. cond. of p-doped substituted polythiophenes)
- IT 7553-56-2, Iodine, uses 14946-92-0, Iron tetrachloride
(dopant; temp.-dependent elec. cond. of p-doped substituted polythiophenes)
- IT 110134-47-9, Poly(3-hexyl-2,5-thiophenediyl) 135899-67-1,
3-Thiophenepropanesulfonic acid homopolymer 216318-88-6,
Poly(3-methyl-2,5-thiophenediyl)
(doped; temp.-dependent elec. cond. of p-doped substituted polythiophenes)
- IT 126213-50-1P
(in prepn. of dichloro thiophene monomer)
- IT 163359-60-2P **225518-50-3P**
(iodine- and iron tetrachloride-doped; temp.-dependent elec. cond. of p-doped substituted polythiophenes)
- IT **225518-49-0P**
(monomer; temp.-dependent elec. cond. of p-doped substituted polythiophenes)

L25 ANSWER 6 OF 6 HCA COPYRIGHT 2005 ACS on STN

82:170765 Methylenedioxyhetarenes. 2. Reactions of diethyl
3,4-methylenedioxy-2,5-thiophenedicarboxylate. Dallacker, Franz;
Mues, Volker (Inst. Org. Chem., Tech. Hochsch. Aachen, Aachen, Fed.
Rep. Ger.). Chemische Berichte, 108(2), 576-81 (German) 1975.
CODEN: CHBEAM. ISSN: 0009-2940. OTHER SOURCES: CASREACT 82:170765.

GI For diagram(s), see printed CA Issue.

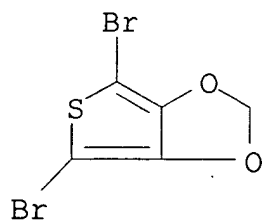
AB The sym. thiophene deriv. I (R = R1 = CO2Et) (II) was treated with
excess alc. KOH, N2H4.H2O, and Br at pH 7.0 to give .apprx.100% I (R
= R1 = CO2H) (III), 79% I (R = R1 = CONHNH2) (IV), and extremely
light- and air-sensitive I (R = R1 = Br) (V), resp. III was
esterified to give I (R = R1 = CO2Me) or chlorinated and aminated,
e.g. with NH3, to give I (R = R1 = CONH2) (VI). IV was condensed
with piperonal to yield the piperonylidene deriv. I (R = R1 =
CONHN:CHC6H3O2CH2-3,4) and V converted into I (R = R1 = iodo).
Boiling VI and POCl3 gave 54% I (R = R1 = CN), which with H2S in
pyridine-Et3N gave 100% I (R = R1 = CSNH2).

IT **55370-18-8P 55370-19-9P**

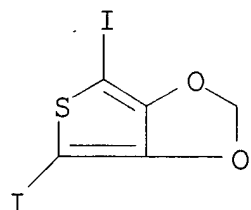
(prepn. of)

RN 55370-18-8 HCA

CN Thieno[3,4-d]-1,3-dioxole, 4,6-dibromo- (9CI) (CA INDEX NAME)



RN 55370-19-9 HCA
 CN Thieno[3,4-d]-1,3-dioxole, 4,6-diiodo- (9CI) (CA INDEX NAME)



IT 55370-05-3
 (bromination and hydrazinolysis and hydrolysis of)
 IT 55370-20-2P
 (prepn. and decarboxylation and esterification and reaction with
 thionyl chloride)
 IT 55370-12-2P 55370-24-6P
 (prepn. and dehydration of)
 IT 55370-26-8P 55370-28-0P
 (prepn. and hydrolysis of)
 IT 55370-11-1P
 (prepn. and reaction with amines)
 IT 55370-06-4P
 (prepn. and reaction with bromine and methanol and thionyl
 chloride)
 IT 55370-08-6P
 (prepn. and reaction with piperonal)
 IT 55370-30-4P
 (prepn. and reaction with sodium sulfide)
 IT 55370-07-5P 55370-09-7P 55370-10-0P 55370-13-3P 55370-14-4P
 55370-15-5P 55370-16-6P 55370-17-7P **55370-18-8P**
55370-19-9P 55370-21-3P 55370-22-4P 55370-23-5P
 55370-25-7P 55370-27-9P 55370-29-1P 55370-31-5P
 (prepn. of)
 IT 120-57-0
 (reaction of, with (methylenedioxy)thiophenecarbohydrazide)
 IT 100-61-8
 (reaction of, with (methylenedioxy)thiophenedicarboxylic

acid)
IT 30525-89-4
 (reaction of, with dibromobutanediol)
IT 14396-65-7
 (reaction of, with formaldehyde)
IT 110-89-4, reactions
 (with (methylenedioxy)thiophenedicarboxylic acid)

=> d 127 1-26 cbib abs hitstr it

L27 ANSWER 1 OF 26 HCA COPYRIGHT 2005 ACS on STN

141:380500 Spray Coatable Electrochromic Dioxothiophene Polymers with High Coloration Efficiencies. Reeves, Benjamin D.; Grenier, Christophe R. G.; Argun, Avni A.; Cirpan, Ali; McCarley, Tracy D.; Reynolds, John R. (Department of Chemistry, Center for Macromolecular Science and Engineering, University of Florida, Gainesville, FL, 32611-7200, USA). *Macromolecules*, 37(20), 7559-7569 (English) 2004. CODEN: MAMOBX. ISSN: 0024-9297. Publisher: American Chemical Society.

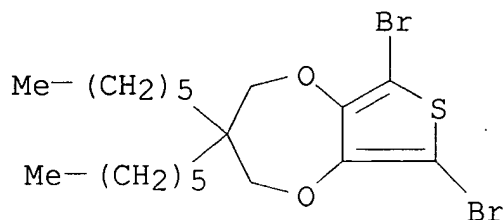
AB Four new disubstituted propylenedioxythiophene polymers have been synthesized by Grignard metathesis on the 1-5 g scale. All polymers were found to be sol. in chloroform, methylene chloride, toluene, and THF and were fully structurally characterized having GPC detd. no.-av. mol. wts. ranging from 33000 to 47000 g mol⁻¹. Dil. polymer solns. in toluene exhibited strong red fluorescence with moderate quantum efficiencies from 0.38 to 0.50. Homogeneous thin films were formed by electropolymerization and spray casting polymer solns. onto ITO coated glass slides at thicknesses of ca. 150 nm. The films were electroactive, switching from a dark blue-purple to a transmissive sky blue upon p-doping, often with subsecond switching times, and high electrochromic contrast luminance changes (% ΔY) of 40-70%. These studies revealed that the branched derivs., [poly(3,3-bis(2-ethylhexyl)-3,4-dihydro-2H-thieno[3,4-b][1,4]dioxepine)] and [poly(6,8-dibromo-3,3-bis(2-ethylhexyloxymethyl)-3,4-dihydro-2H-thieno[3,4-b][1,4]dioxepine)], gave an electrochem. response and assocd. color change over a much smaller voltage range in comparison to the linear chain substituted derivs., [poly(3,3-diethyl-3,4-dihydro-2H-thieno[3,4-b][1,4]dioxepine)] and [poly(3,3-bis(octadecyloxymethyl)-3,4-dihydro-2H-thieno[3,4-b][1,4]dioxepine)]. Composite coloration efficiency values were found up to 1365 cm²/C; this was considerably larger than values obtained from previously studied alkylenedioxythiophene based polymers (.apprx.375 cm²/C).

IT 700817-04-5P 700817-06-7P 700817-08-9P
700817-10-3P

(monomer; prepn. and electrooptical properties of spray coatable electrochromic dioxothiophene polymers)

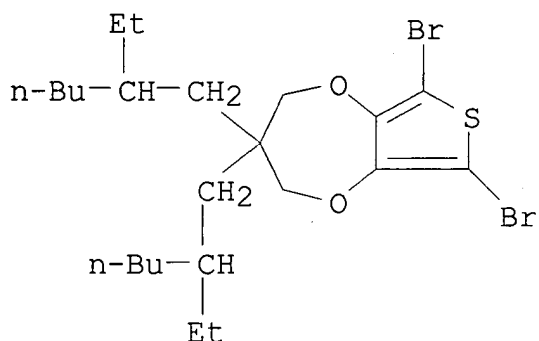
RN 700817-04-5 HCA

CN 2H-Thieno[3,4-b][1,4]dioxepin, 6,8-dibromo-3,3-dihexyl-3,4-dihydro-
(9CI) (CA INDEX NAME)



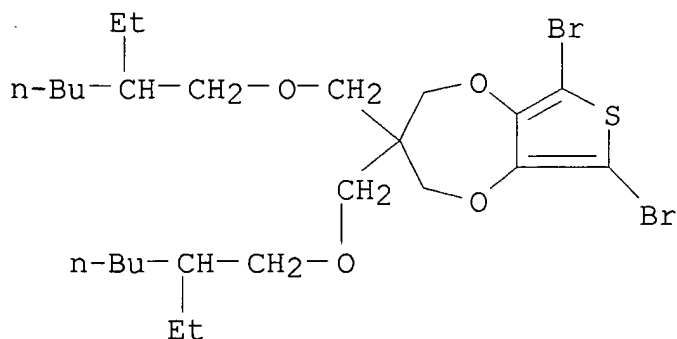
RN 700817-06-7 HCA

CN 2H-Thieno[3,4-b][1,4]dioxepin, 6,8-dibromo-3,3-bis(2-ethylhexyl)-3,4-dihydro- (9CI) (CA INDEX NAME)



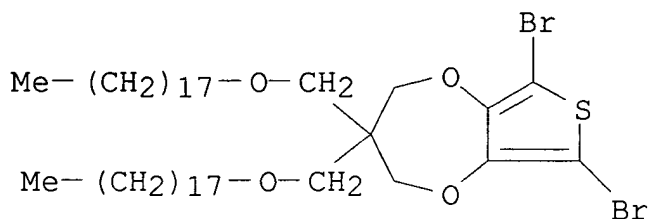
RN 700817-08-9 HCA

CN 2H-Thieno[3,4-b][1,4]dioxepin, 6,8-dibromo-3,3-bis[[(2-ethylhexyl)oxy)methyl]-3,4-dihydro- (9CI) (CA INDEX NAME)



RN 700817-10-3 HCA

CN 2H-Thieno[3,4-b][1,4]dioxepin, 6,8-dibromo-3,4-dihydro-3,3-bis[(octadecyloxy)methyl]- (9CI) (CA INDEX NAME)



- IT Polymerization
(Grignard; prepn. and electrooptical properties of spray coatable electrochromic dioxothiophene polymers)
- IT Polymerization
(electrochem.; prepn. and electrooptical properties of spray coatable electrochromic dioxothiophene polymers)
- IT Band gap
(optical; prepn. and electrooptical properties of spray coatable electrochromic dioxothiophene polymers)
- IT Conducting polymers
(polythiophenes; prepn. and electrooptical properties of spray coatable electrochromic dioxothiophene polymers)
- IT Electrochromism
Luminescence, electroluminescence
Redox potential
(prepn. and electrooptical properties of spray coatable electrochromic dioxothiophene polymers)
- IT Electrooptical effect
(switching; prepn. and electrooptical properties of spray coatable electrochromic dioxothiophene polymers)
- IT 104-76-7, 2-Ethyl-1-hexanol 105-53-3, Diethyl malonate 111-25-1, Hexyl bromide 112-92-5, 1-Octadecanol 3296-90-0, 2,2-Di(bromomethyl)-1,3-diol 18908-66-2, 2-Ethylhexyl bromide 51792-34-8, 3,4-Dimethoxythiophene
(monomer synthesis; prepn. and electrooptical properties of spray coatable electrochromic dioxothiophene polymers)
- IT 54662-33-8P 634591-75-6P 634591-77-8P 700816-90-6P 701209-98-5P
(monomer synthesis; prepn. and electrooptical properties of spray coatable electrochromic dioxothiophene polymers)
- IT 700816-98-4P 700817-00-1P **700817-04-5P**
700817-06-7P 700817-08-9P 700817-10-3P
(monomer; prepn. and electrooptical properties of spray coatable electrochromic dioxothiophene polymers)
- IT 700817-12-5P 700817-14-7P 700817-16-9P 700817-18-1P 783322-80-5P 783322-81-6P 783322-82-7P 783322-83-8P
(prepn. and electrooptical properties of spray coatable electrochromic dioxothiophene polymers)

L27 ANSWER 2 OF 26 HCA COPYRIGHT 2005 ACS on STN

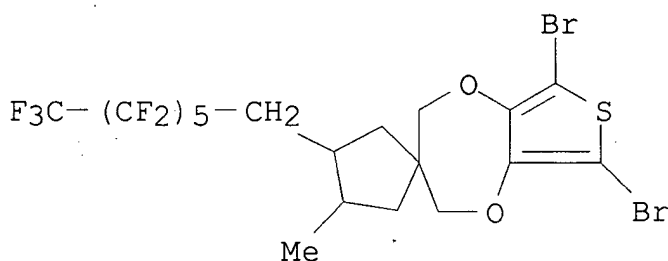
141:314660 Synthesis and polymerization of perfluoroalkylated 3,4-propylenedioxythiophene. Dong, Jian-Hai; Meng, Wei-Dong; Qing, Feng-Ling (Coll. Chem. Chem. Eng., Donghua Univ., Shanghai, 200051, Peop. Rep. China). ARKIVOC (Gainesville, FL, United States) (9), 9-14 (English) 2004. CODEN: AGFUAR. URL: <http://www.arkat-usa.org/ark/journal/2004/Yuan/CY-1037L/CY-1037L.pdf> Publisher: Arkat USA Inc..

AB A novel monomer, perfluoroalkylated 3,4-propylenedioxythiophene, was prepd. by trans-etherification reaction between 3,4-dimethoxythiophene and perfluoroalkylated cycloalkylpropane-1,3-diol. Bromination of monomer followed by a Grignard metathesis coupling reaction provided perfluoroalkylated poly(3,4-propylenedioxythiophene). This polymer was quite insol. in any known solvent.

IT **768400-95-9P**
(multi-step prepn. of perfluoroalkylated propylenedioxythiophene monomer and its bromination followed by Grignard metathesis coupling polymn.)

RN 768400-95-9 HCA

CN Spiro[cyclopentane-1,3'-(4'H)-[2H]thieno[3,4-b][1,4]dioxepin], 6',8'-dibromo-3-methyl-4-(2,2,3,3,4,4,5,5,6,6,7,7,7-tridecafluoroheptyl)- (9CI) (CA INDEX NAME)



IT Polymerization
(Grignard, metathetic; multi-step prepn. of perfluoroalkylated propylenedioxythiophene monomer and its bromination followed by Grignard metathesis coupling polymn.)

IT Polymerization
(metathetic, Grignard; multi-step prepn. of perfluoroalkylated propylenedioxythiophene monomer and its bromination followed by Grignard metathesis coupling polymn.)

IT 3195-24-2P, Diethyl 2,2-diallylmalonate
(cyclization of; multi-step prepn. of perfluoroalkylated propylenedioxythiophene monomer and its bromination followed by Grignard metathesis coupling polymn.)

IT 768400-93-7P

- (cycloaddn. of; multi-step prepn. of perfluoroalkylated propylenedioxythiophene monomer and its bromination followed by Grignard metathesis coupling polymn.)
- IT 105-53-3, Diethyl malonate 106-95-6, Allyl bromide, reactions 355-43-1, Perfluorohexyl iodide 51792-34-8, 3,4-Dimethoxythiophene (multi-step prepn. of perfluoroalkylated propylenedioxythiophene monomer and its bromination followed by Grignard metathesis coupling polymn.)
- IT 768400-94-8P **768400-95-9P** (multi-step prepn. of perfluoroalkylated propylenedioxythiophene monomer and its bromination followed by Grignard metathesis coupling polymn.)
- IT 768400-96-0P (multi-step prepn. of perfluoroalkylated propylenedioxythiophene monomer and its bromination followed by Grignard metathesis coupling polymn.)
- IT 169893-13-4P (redn. of; multi-step prepn. of perfluoroalkylated propylenedioxythiophene monomer and its bromination followed by Grignard metathesis coupling polymn.)

L27 ANSWER 3 OF 26 HCA COPYRIGHT 2005 ACS on STN

141:89456 Copolymers of 3,4-Ethylenedioxythiophene and of Pyridine Alternated with Fluorene or Phenylene Units: Synthesis, Optical Properties, and Devices. Aubert, Pierre-Henri; Knipper, Martin; Groenendaal, Lambertus; Lutsen, Laurence; Manca, Jean; Vanderzande, Dirk (IMOMEC Division, IMEC, Diepenbeek, B-3590, Belg.). Macromolecules, 37(11), 4087-4098 (English) 2004. CODEN: MAMOBX. ISSN: 0024-9297. Publisher: American Chemical Society.

AB We report the synthesis of four conjugated copolymers based on alkylated fluorene or phenylene units which band gap is tuned by the regular insertion of an electron-donating or electron-withdrawing unit, (3,4-ethylenedioxy)thiophene and pyridine, resp. The (AB)_n regular sequence is achieved by Suzuki polycondensation reactions. The characterization of the copolymers by size exclusion chromatog. reveals chains lengths of about 20-30 repeat units (40-60 rings), leading to a good processability for potential optical applications. The 1:1 ratio between the two units improves the soly. of the material in common org. solvents, allowing for physicochem. characterizations. Raman and FT-IR expts. indicate that the electronic structure of the backbone is rather benzenic in the neutral (undoped) state, as opposed to a quinoic oxidized structure. All copolymers exhibit interesting electrochromic properties as attested by cyclic voltammetry and UV-vis expts. They reversibly switch among the entire visible spectra, which is of particular importance for display applications. Moreover, the EDOT-based copolymers strongly absorb in the NIR window (1200 nm up to 3000 nm) with some potential electrochromic applications related to this

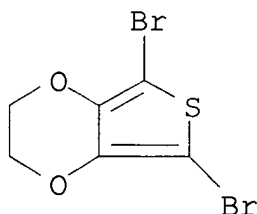
spectral window. Light-emitting diodes were fabricated using these copolymers as active layer. To improve hole and electron injection, the active layer was sandwiched between a ITO/PEDOT:PSSA/copolymer/Ba/Al. The emitting properties were studied on the base of photoluminescence (PL) and electroluminescence (EL) expts. The spectral emission varies from blue-green to yellow, depending on the compn. of the copolymers.

IT 174508-31-7P

(monomer; prepn. and optical properties of and LEDs from copolymers prepd. from dibromoethylenedioxythiophene or dibromopyridine and contg. fluorene or phenylene units)

RN 174508-31-7 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro- (9CI) (CA INDEX NAME)



IT Polymers, preparation

(conjugated; prepn. and optical properties of and LEDs from copolymers prepd. from dibromoethylenedioxythiophene or dibromopyridine and contg. fluorene or phenylene units)

IT Doping

(electrochem.; prepn. and optical properties of and LEDs from copolymers prepd. from dibromoethylenedioxythiophene or dibromopyridine and contg. fluorene or phenylene units)

IT Conduction electrons

(injection; prepn. and optical properties of and LEDs from copolymers prepd. from dibromoethylenedioxythiophene or dibromopyridine and contg. fluorene or phenylene units)

IT Band gap

(optical; prepn. and optical properties of and LEDs from copolymers prepd. from dibromoethylenedioxythiophene or dibromopyridine and contg. fluorene or phenylene units)

IT Band gap

Electrochromism

Electroluminescent devices

Electronic structure

Glass substrates

Glass transition temperature

HOMO (molecular orbital)

IR spectra

LUMO (molecular orbital)

Luminescence

Luminescence, electroluminescence

Polymerization

Polymerization catalysts

Raman spectra

Redox potential

Redox reaction

Thermal stability

UV and visible spectra

(prepn. and optical properties of and LEDs from copolymers prepd. from dibromoethylenedioxythiophene or dibromopyridine and contg. fluorene or phenylene units)

IT 9003-53-6D, sulfonated

(PSS; prepn. and optical properties of and LEDs from copolymers prepd. from dibromoethylenedioxythiophene or dibromopyridine and contg. fluorene or phenylene units)

IT 7429-90-5, Aluminum, uses 7440-39-3, Barium, uses

(electrode; prepn. and optical properties of and LEDs from copolymers prepd. from dibromoethylenedioxythiophene or dibromopyridine and contg. fluorene or phenylene units)

IT 67399-94-4P, 1,4-Dioctyloxybenzene 123863-99-0P,
9,9-Dioctylfluorene 156028-40-9P, 1,4-Dibromo-2,5-

dioctyloxybenzene 198964-46-4P, 2,7-Dibromo-9,9-dioctylfluorene (intermediate in monomer prepn.; prepn. and optical properties of and LEDs from copolymers prepd. from dibromoethylenedioxythiophene or dibromopyridine and contg. fluorene or phenylene units)

IT 174508-31-7P 196207-58-6P 406461-51-6P 457931-26-9P

(monomer; prepn. and optical properties of and LEDs from copolymers prepd. from dibromoethylenedioxythiophene or dibromopyridine and contg. fluorene or phenylene units)

IT 14221-01-3, Pd(PPh₃)₄

(polymn. catalysts; prepn. and optical properties of and LEDs from copolymers prepd. from dibromoethylenedioxythiophene or dibromopyridine and contg. fluorene or phenylene units)

IT 50926-11-9, ITO 126213-51-2, PEDOT

(prepn. and optical properties of and LEDs from copolymers prepd. from dibromoethylenedioxythiophene or dibromopyridine and contg. fluorene or phenylene units)

IT 287924-59-8P 287924-60-1P 294637-16-4P 473914-21-5P

633290-76-3P 716377-30-9P 716377-31-0P 716377-32-1P

716377-33-2P 716377-34-3P

(prepn. and optical properties of and LEDs from copolymers prepd. from dibromoethylenedioxythiophene or dibromopyridine and contg. fluorene or phenylene units)

IT 86-73-7, Fluorene 111-83-1, Octyl bromide 123-31-9,

Hydroquinone, reactions 61676-62-8, 2-Isopropoxy-4,4,5,5-

tetramethyl-[1,3,2]dioxaborolane 126213-50-1

(reactant in monomer prepn.; prepn. and optical properties of and LEDs from copolymers prepd. from dibromoethylenedioxythiophene or dibromopyridine and contg. fluorene or phenylene units)

L27 ANSWER 4 OF 26 HCA COPYRIGHT 2005 ACS on STN

141:39122 Synthetic methodology toward new propylenedioxythiophene polymers. Reeves, Benjamin D.; Grenier, Christophe R. G.; Argun, Avni A.; Cirpan, Ali; Cunningham, Garry B.; McCarley, Tracy D.; Reynolds, John R. (Department of Chemistry, Center for Macromolecular Science and Engineering, University of Florida, Gainesville, FL, 32611, USA). Polymer Preprints (American Chemical Society, Division of Polymer Chemistry), 45(1), 284 (English) 2004. CODEN: ACPPAY. ISSN: 0032-3934. Publisher: American Chemical Society, Division of Polymer Chemistry.

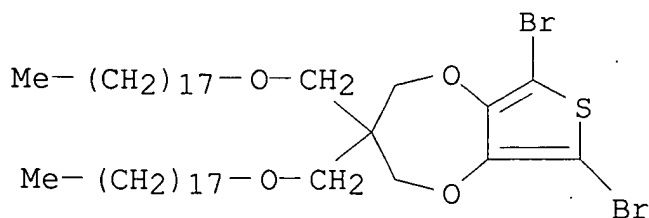
AB An extensive family of dioxythiophene-based monomers by Williamson etherification, transesterification, and Mitsunobu chem. has been successfully synthesized by our group, however, the routes developed are not efficient when synthesizing monomers with large substituents. Therefore, a new synthetic methodol. has been employed to access monomers with large nonpolar derivs. First, 3,4-dimethoxythiophene is subject to a transesterification reaction with 2,2-bis(bromomethyl)-1,3-propanediol. The bromomethyl derivatized ProDOT then undergoes a Williamson etherification with octadecanol and the octadecyl deriv. was then brominated with NBS followed by polymn. by Grignard metathesis. The resulting polymer after purifn. by fractionation was characterized by NMR, GPC, MALDI-TOF, X-ray powder diffraction, DSC, and TGA. The polymer was highly sol. in org. solvents, which allowed the spray casting of thin films from soln. and the films were then electrochromically characterized and incorporated into dual polymer electrochromic devices. Also, a polymer soln. in toluene gave a relatively high fluorescence quantum efficiency with a value of 0.40.

IT 700817-10-3P

(synthesis of propylenedioxythiophene-based monomer for polymers thereof)

RN 700817-10-3 HCA

CN 2H-Thieno[3,4-b][1,4]dioxepin, 6,8-dibromo-3,4-dihydro-3,3-bis[(octadecyloxy)methyl]- (9CI) (CA INDEX NAME)



- IT Polymerization
(Grignard; synthesis of propylenedioxythiophene polymers and fluorescence thereof)
- IT Alkoxylation
(Williamson; synthesis of propylenedioxythiophene-based monomer for polymers thereof)
- IT Polymerization
(metathetic; synthesis of propylenedioxythiophene polymers and fluorescence thereof)
- IT Fluorescence
(of propylenedioxythiophene polymers)
- IT Conducting polymers
(polythiophenes; synthesis of propylenedioxythiophene polymers and fluorescence thereof)
- IT Etherification
(transesterification; synthesis of propylenedioxythiophene-based monomer for polymers thereof)
- IT 3296-90-0 51792-34-8
(in synthesis of propylenedioxythiophene-based monomer for polymers thereof)
- IT 634591-77-8P 701209-98-5P
(in synthesis of propylenedioxythiophene-based monomer for polymers thereof)
- IT 700817-18-1P
(synthesis of propylenedioxythiophene polymers and fluorescence thereof)
- IT **700817-10-3P**
(synthesis of propylenedioxythiophene-based monomer for polymers thereof)

L27 ANSWER 5 OF 26 HCA COPYRIGHT 2005 ACS on STN

141:24056 Solution processable and electrochromic dioxythiophene-based polymers. Reeves, Benjamin D.; Grenier, Christophe R. G.; Argun, Avni A.; Cirpan, Ali; McCarley, Tracy D.; Reynolds, John R. (Department of Chemistry, Center for Macromolecular Science and Engineering, University of Florida, Gainesville, FL, 32611, USA). Polymer Preprints (American Chemical Society, Division of Polymer Chemistry), 45(1), 180 (English) 2004. CODEN: ACPPAY. ISSN: 0032-3934. Publisher: American Chemical Society, Division of Polymer Chemistry.

AB This work presents the development of a family of sol. processable disubstituted propylenedioxythiophenes and an anal. of their electrochromic properties. 2,5-Dibromo derivatized dioxythiophene monomers underwent Grignard metathesis polymn. to afford org. sol. neutral polymers. Polymers were characterized by NMR, GPC, MALDI-TOF, X-ray powder diffraction, TGA, and DSC. Mol. wt. characterization by GPC vs. polystyrene stds. indicated no. av. mol.

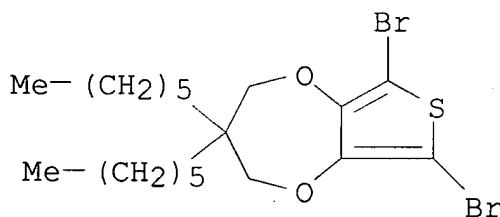
wts. between 7-40 kg/mol. MALDI-TOF studies were performed which gave a set of dominant peaks sep'd. by 322 amu, corresponding to the mol. wt. of the monomer repeat unit. Thin films were processed by spray casting polymer solns. onto a working electrode. Spectroelectrochem., colorimetry, and composite coloration efficiencies studies show that the spray cast polymers have the same contrast ratio and switching speeds as the electrodeposited films of the same thickness. The composite coloration efficiency values for this family are two to three times larger than previously obsd. for electrodeposited dioxothiophene polymers.

IT 700817-04-5P 700817-06-7P 700817-08-9P
700817-10-3P

(monomer; in prepn. of soln. processable and electrochromic dioxothiophene-based polymers)

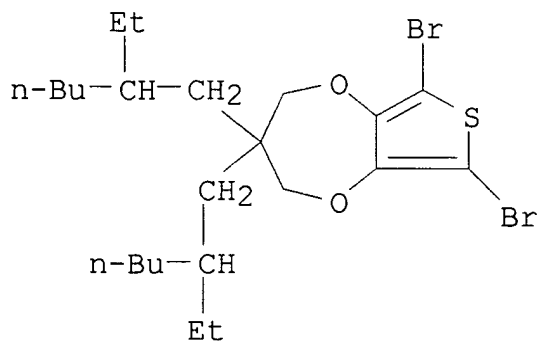
RN 700817-04-5 HCA

CN 2H-Thieno[3,4-b][1,4]dioxepin, 6,8-dibromo-3,3-dihexyl-3,4-dihydro- (9CI) (CA INDEX NAME)



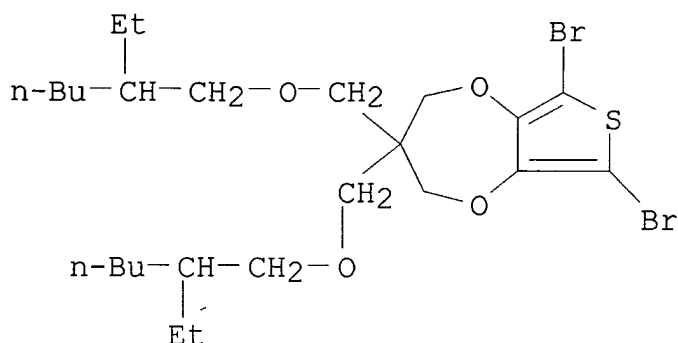
RN 700817-06-7 HCA

CN 2H-Thieno[3,4-b][1,4]dioxepin, 6,8-dibromo-3,3-bis(2-ethylhexyl)-3,4-dihydro- (9CI) (CA INDEX NAME)



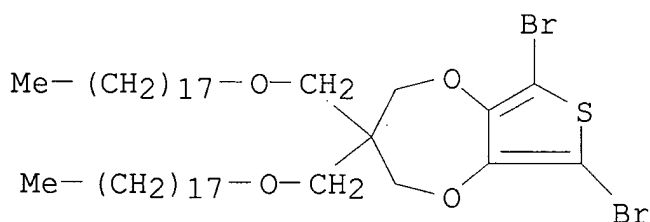
RN 700817-08-9 HCA

CN 2H-Thieno[3,4-b][1,4]dioxepin, 6,8-dibromo-3,3-bis[(2-ethylhexyl)oxy)methyl]-3,4-dihydro- (9CI) (CA INDEX NAME)



RN 700817-10-3 HCA

CN 2H-Thieno[3,4-b][1,4]dioxepin, 6,8-dibromo-3,4-dihydro-3,3-bis[(octadecyloxy)methyl]- (9CI) (CA INDEX NAME)



- IT Alkoxylation
(Williamson; in prepn. of monomers for soln. processable and electrochromic dioxothiophene-based polymers)
- IT Bromination
- IT Transesterification
(in prepn. of monomers for soln. processable and electrochromic dioxothiophene-based polymers)
- IT Polymerization
(metathetic; in prepn. of soln. processable and electrochromic dioxothiophene-based polymers)
- IT Optical switching
(of electrochromic dioxothiophene-based polymers)
- IT Molecular weight
(of soln. processable and electrochromic dioxothiophene-based polymers)
- IT Conducting polymers
(polythiophenes; prepn. of soln. processable and electrochromic dioxothiophene-based polymers)
- IT Electrochromic materials
(prepn. of soln. processable and dioxothiophene-based polymers for electrochromic materials)
- IT 128-08-5, N-Bromosuccinimide

- (in prepn. of monomers for soln. processable and electrochromic dioxothiophene-based polymers)
- IT 51792-34-8, 3,4-Dimethoxythiophene 54662-33-8 57355-20-1
700816-90-6 700816-93-9
(in prepn. of soln. processable and electrochromic dioxothiophene-based polymers)
- IT 634591-75-6P 634591-77-8P 700816-98-4P 700817-00-1P
(in prepn. of soln. processable and electrochromic dioxothiophene-based polymers)
- IT 700817-04-5P 700817-06-7P 700817-08-9P
700817-10-3P
(monomer; in prepn. of soln. processable and electrochromic dioxothiophene-based polymers)
- IT 700817-12-5P 700817-14-7P 700817-16-9P 700817-18-1P
(prepn. of soln. processable and electrochromic dioxothiophene-based polymers)

L27 ANSWER 6 OF 26 HCA COPYRIGHT 2005 ACS on STN

140:77531 Solid-State Synthesis of a Conducting Polythiophene via an Unprecedented Heterocyclic Coupling Reaction. Meng, Hong; Perepichka, Dmitrii F.; Bendikov, Michael; Wudl, Fred; Pan, Grant Z.; Yu, Wenjiang; Dong, Wenjian; Brown, Stuart (Department of Chemistry and Biochemistry and the Exotic Materials Institute, Microfabrication Lab, Department of Physics and Astrophysics, University of California, Los Angeles, CA, 90095-1569, USA). Journal of the American Chemical Society, 125(49), 15151-15162 (English) 2003. CODEN: JACSAT. ISSN: 0002-7863. Publisher: American Chemical Society.

AB Prolonged storage (.apprx.2 yr) or gentle heating (50-80 °C) of cryst. 2,5-dibromo-3,4-ethylenedioxythiophene (DBEDOT) affords a highly conducting, bromine-doped poly(3,4-ethylenedioxythiophene) (PEDOT), as confirmed by solid-state NMR, FTIR, CV, and vis-NIR spectroscopies. The novel solid-state polymn. (SSP) does not occur for 2,5-dichloro-3,4-ethylenedioxythiophene (DCEDOT), and requires a much higher temp. (>130 °C) for 2,5-diiodo-3,4-ethylenedioxythiophene (DIEDOT). X-ray structural anal. of the above dihalothiophenes reveals short Hal...Hal distances between adjacent mols. in DBEDOT and DIEDOT, but not in DCEDOT. The polymn. may also occur in the melt but is significantly slower and leads to poorly conductive material. Detailed studies of the reaction were performed using ESR, DSC, microscopy, and gravimetric analyses. SSP starts on crystal defect sites; it is exothermic by 14 kcal/mol and requires activation energy of .apprx.26 kcal/mol (for DBEDOT). The temp. dependence of the cond. of SSP-PEDOT ($\sigma_{\text{rt}} = 20\text{-}80 \text{ S/cm}$) reveals a slight thermal activation. It can be further increased by a factor of 2 by doping with iodine. Using this approach, thin films of PEDOT with cond. as high as 20 S/cm were fabricated on insulating flexible plastic

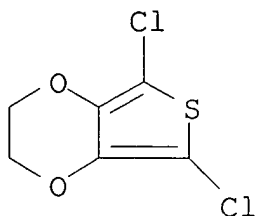
surfaces.

IT 225518-49-0P, 2,5-Dichloro-3,4-Ethylenedioxythiophene
640737-72-0P

(solid-state synthesis of conducting polythiophenes via
unprecedented heterocyclic coupling reaction)

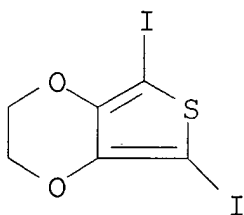
RN 225518-49-0 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dichloro-2,3-dihydro- (9CI) (CA INDEX
NAME)



RN 640737-72-0 HCA

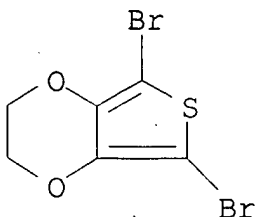
CN Thieno[3,4-b]-1,4-dioxin, 2,3-dihydro-5,7-diiodo- (9CI) (CA INDEX
NAME)



IT 174508-31-7P, 2,5-Dibromo-3,4-Ethylenedioxythiophene
(solid-state synthesis of conducting polythiophenes via
unprecedented heterocyclic coupling reaction)

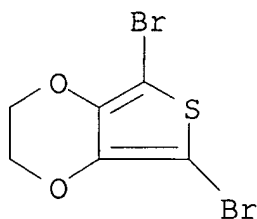
RN 174508-31-7 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro- (9CI) (CA INDEX
NAME)



IT NMR spectroscopy
(carbon-13, solid state; solid-state synthesis of conducting

- polythiophenes via unprecedented heterocyclic coupling reaction)
- IT Polymer morphology
(cryst.; solid-state synthesis of conducting polythiophenes via unprecedented heterocyclic coupling reaction)
- IT Conducting polymers
(polythiophenes; solid-state synthesis of conducting polythiophenes via unprecedented heterocyclic coupling reaction)
- IT Electric conductivity
(solid-state synthesis of conducting polythiophenes via unprecedented heterocyclic coupling reaction)
- IT 225518-49-0P, 2,5-Dichloro-3,4-Ethylenedioxythiophene
640737-72-0P
(solid-state synthesis of conducting polythiophenes via unprecedented heterocyclic coupling reaction)
- IT 350037-71-7P, 2,5-Dibromo-3,4-Ethylenedioxythiophene homopolymer
(solid-state synthesis of conducting polythiophenes via unprecedented heterocyclic coupling reaction)
- IT 174508-31-7P, 2,5-Dibromo-3,4-Ethylenedioxythiophene
640737-73-1P
(solid-state synthesis of conducting polythiophenes via unprecedented heterocyclic coupling reaction)
- IT 109-72-8, n-Butyl lithium, reactions 128-08-5, N-Bromosuccinimide
128-09-6, N-Chlorosuccinimide 1600-27-7, Mercuric acetate
7553-56-2, Iodine, reactions 126213-50-1, 3,4-Ethylenedioxythiophene
(solid-state synthesis of conducting polythiophenes via unprecedented heterocyclic coupling reaction)
- L27 ANSWER 7 OF 26 HCA COPYRIGHT 2005 ACS on STN
- 139:149947 Stable and Soluble Oligo(3,4-ethylenedioxythiophene)s End-Capped with Alkyl Chains. Turbiez, Mathieu; Frere, Pierre; Roncali, Jean (Groupe Systemes Conjugues Lineaires, Laboratoire IMMO, UMR CNRS 6501, Universite d'Angers, Angers, 49000, Fr.). Journal of Organic Chemistry, 68(13), 5357-5360 (English) 2003. CODEN: JOCEAH. ISSN: 0022-3263. Publisher: American Chemical Society.
- AB The synthesis of a new series of stable and sol. EDOT oligomers end-capped with n-hexyl groups is described. Optical and electrochem. results indicate that the synergy between the direct electron-releasing effects of the ethylenedioxy groups and the self-rigidification resulting from intramol. interactions controls to a large extent the HOMO-LUMO gap.
- IT 174508-31-7P, 2,5-Dibromo-3,4-ethylenedioxythiophene
(intermediate; prepn. of, and in reaction with tributylstannylhexyl-EDOT)
- RN 174508-31-7 HCA
- CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro- (9CI) (CA INDEX NAME)



- IT UV absorption
(UV-visible; of oligo(3,4-ethylenedioxythiophene)s end-capped with alkyl chains)
- IT Bathochromic effect
Crystal structure
Cyclic voltammetry
Oxidation potential
Solubility
(of oligo(3,4-ethylenedioxythiophene)s end-capped with alkyl chains)
- IT 569665-35-6P
(dimer; synthesis and properties of oligo(3,4-ethylenedioxythiophene)s end-capped with alkyl chains)
- IT 128-08-5, NBS
(in reaction with EDOT or bisEDOT)
- IT 126213-50-1, 3,4-Ethylenedioxythiophene
(in reaction with bromohexane)
- IT 25495-91-4, Bromohexane
(in reaction with ethylenedioxythiophene or bisethylenedioxythiophene)
- IT 1461-22-9, Tributylstannyl chloride
(in reaction with hexylethylenedioxythiophene)
- IT 569665-37-8P
(intermediate; prepn. of, and in reaction with dibromo-EDOT or dibromo-bisEDOT)
- IT 569665-30-1P
(intermediate; prepn. of, and in reaction with tributylstannyl chloride or in dimerization)
- IT **174508-31-7P**, 2,5-Dibromo-3,4-ethylenedioxythiophene
287924-56-5P
(intermediate; prepn. of, and in reaction with tributylstannylhexyl-EDOT)
- IT 569665-32-3P
(prepn. of)
- IT 195602-17-6
(reaction with bromohexane in synthesis of dimer)
- IT 569665-42-5P
(tetramer; synthesis and properties of oligo(3,4-

ethylenedioxythiophene)s end-capped with alkyl chains)
IT 569665-39-0P
(trimer; synthesis and properties of oligo(3,4-
ethylenedioxythiophene)s end-capped with alkyl chains)

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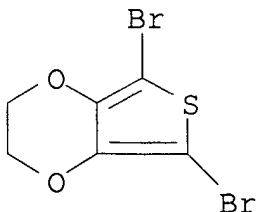
138:304877 3,4-Ethylenedioxy-substituted bithiophene-alt-thiophene-S,S-dioxide regular copolymers. Synthesis and conductive, magnetic and luminescence properties.. Berlin, Anna; Zotti, Gianni; Zecchin, Sandro; Schiavon, Gilberto; Cocchi, Massimo; Virgili, Dalia; Sabatini, Cristiana (Istituto CNR di Scienze e Tecnologie Molecolari, Milan, 20133, Italy). Journal of Materials Chemistry, 13(1), 27-33 (English) 2003. CODEN: JMACEP. ISSN: 0959-9428. Publisher: Royal Society of Chemistry.

AB Polyconjugated regular bithiophene-alt-thiophene-S,S-dioxide copolymers were produced by anodic coupling of variously 3,4-ethylenedioxy-substituted 2,5-bis(2-thienyl)thiophene-S,S-dioxide. The polymers were characterized by cyclic voltammetry, FTIR reflection-absorption and UV-vis spectroscopy, MALDI-TOF mass spectroscopy, electrochem. quartz crystal microbalance, in situ ESR and in situ cond. techniques, photo- and electro-luminescence measurements. The regular alternation of electron-rich and -poor thiophene rings in the polymer chain operated by the ethylenedioxy and S,S-dioxide moieties produces a finite window of cond. Alkyl-protection of the β -positions of the thiophene-S,S-dioxide ring gave low-defect and sol. oligomers which were investigated in single-layer org. light-emitting devices (OLEDs). Photoluminescence quantum efficiency of .apprx.1% and external electroluminescence quantum efficiencies of 0.01% photon/electron at a luminance of 100 cd m⁻² were obtained.

IT 174508-31-7, 2,5-Dibromo-3,4-(ethylenedioxy)thiophene
(oxidn. of)

RN 174508-31-7 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro- (9CI) (CA INDEX NAME)

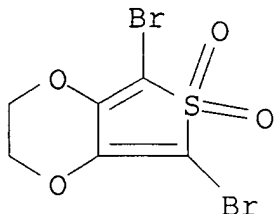


IT 511286-87-6P

(prepn. and reaction with (tributylstannyl)thiophene)

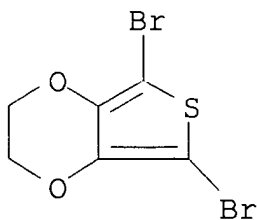
RN 511286-87-6 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro-, 6,6-dioxide
(9CI) (CA INDEX NAME)



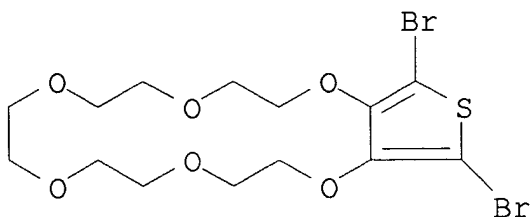
- IT Oxidation potential
Reduction potential
(of ethylenedioxy-substituted bis(thienyl)thiophene dioxide monomers and polymers)
- IT Electric conductivity
Luminescence
Luminescence, electroluminescence
(prepn. and conductive, magnetic and luminescence properties of ethylenedioxy-substituted bithiophene-alt-thiophene dioxide polymers)
- IT Electroluminescent devices
(single-layer electroluminescence devices prepd. from ethylenedioxy-substituted bithiophene-alt-thiophene dioxide polymers)
- IT Polycarbonates, properties
(single-layer electroluminescence devices prepd. from ethylenedioxy-substituted bithiophene-alt-thiophene dioxide polymers and)
- IT 25037-45-0, Bisphenol A polycarbonate
(assumed monomers; single-layer electroluminescence devices prepd. from ethylenedioxy-substituted bithiophene-alt-thiophene dioxide polymers and)
- IT **174508-31-7**, 2,5-Dibromo-3,4-(ethylenedioxy)thiophene
174509-52-5
(oxidn. of)
- IT 511286-88-7P 511286-89-8P 511286-90-1P 511286-91-2P
511286-92-3P
(prepn. and conductive, magnetic and luminescence properties of)
- IT 511286-81-0P 511286-82-1P 511286-83-2P 511286-84-3P
511286-85-4P
(prepn. and polymn. of)
- IT 511286-86-5P
(prepn. and reaction with (tributylstannyl)(ethylenedioxy)thiophene)
- IT **511286-87-6P**
(prepn. and reaction with (tributylstannyl)thiophene)

- IT 89088-95-9, 2,5-Dibromothiophene-1,1-dioxide
(reaction with (tributylstannyl)(ethylenedioxy)thiophene)
- IT 175922-79-9, 2-(Tributylstannyl)-3,4-(ethylenedioxy)thiophene
(reaction with dibromothiophene dioxide)
- IT 24936-68-3, Bisphenol A polycarbonate, sru, properties 65181-78-4,
N,N'-Diphenyl-N,N'-bis(3-methylphenyl)-1,1'-biphenyl-4,4'-diamine
(single-layer electroluminescence devices prepd. from
ethylenedioxy-substituted bithiophene-alt-thiophene dioxide
polymers and)
- L27 ANSWER 9 OF 26 HCA COPYRIGHT 2005 ACS on STN
- 138:288055 Facile solid-state synthesis of highly conducting
poly(ethylenedioxythiophene). Meng, Hong; Perepichka, Dmitrii F.;
Wudl, Fred (Department of Chemistry and Biochemistry and Exotic
Materials Institute, University of California, Los Angeles, CA,
90095-1569, USA). Angewandte Chemie, International Edition, 42(6),
658-661 (English) 2003. CODEN: ACIEF5. ISSN: 1433-7851.
Publisher: Wiley-VCH Verlag GmbH & Co. KGaA.
- AB The prepn. of PEDOT by catalyst-free coupling polymn. of
2,5-dibromo-3,4-ethylenedioxythiophene in the solid state at
accelerated temps. (60, 80, and 120°) is reported. The cond.
of polymer films on plastic and glass substrate was examd. Crystal
structure data for the monomer are presented.
- IT 174508-31-7, 2,5-Dibromo-3,4-ethylenedioxythiophene
(structure and solid-state polymn. of
dibromoethylenedioxythiophene)
- RN 174508-31-7 HCA
- CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro- (9CI) (CA INDEX
NAME)



- IT Polymer morphology
(cryst.; solid-state polymn. of dibromoethylenedioxythiophene and
cond. of poly(ethylenedioxythiophene))
- IT Crystal structure
(of 2,5-dibromo-3,4-ethylenedioxythiophene)
- IT Conducting polymers
Electric conductivity
(solid-state polymn. of dibromoethylenedioxythiophene and cond.
of poly(ethylenedioxythiophene))

- IT 163359-60-2P, 2,5-Dibromo-3,4-ethylenedioxythiophene homopolymer,
SRU 350037-71-7P, 2,5-Dibromo-3,4-ethylenedioxythiophene
homopolymer
(solid-state polymn. of dibromoethylenedioxythiophene and cond.
of poly(ethylenedioxythiophene))
- IT **174508-31-7**, 2,5-Dibromo-3,4-ethylenedioxythiophene
(structure and solid-state polymn. of
dibromoethylenedioxythiophene)
- L27 ANSWER 10 OF 26 HCA COPYRIGHT 2005 ACS on STN
- 138:188206 EQCM analysis of the alkali metal ion coordination properties
of novel poly(thiophene)s 3,4-functionalized with crown-ether
moieties. Berlin, A.; Zotti, G.; Zecchin, S.; Schiavon, G.
(Istituto CNR di Scienze e Tecnologie Molecolari, Milan, 20133,
Italy). Synthetic Metals, 131(1-3), 149-160 (English) 2002. CODEN:
SYMEDZ. ISSN: 0379-6779. Publisher: Elsevier Science B.V..
- AB New thiophenes carrying 18-crown-6-ether ring directly linked to the
3- and 4-positions of the thiophene ring were synthesized and
polymd. by anodic coupling in acetonitrile. The polymers were
characterized by cyclic voltammetry (CV), UV-Vis and FTIR
spectroscopy, matrix-assisted laser desorption ionization (MALDI)
mass spectroscopy and in situ cond. Electrochem. quartz crystal
microbalance (EQCM) anal. of the alkali metal coordination ability
of the 18-crown-6-ether polymer films in acetonitrile has evidenced
that the coordination consts. (e.g. 20-80 M⁻¹ for Na⁺) are ca. two
orders of magnitude lower than those of polythiophenes bearing the
crown substituents pendant from the polythiophene backbone. The
result has been ascribed both to electronic and solid-state effects
of the conjugated polythiophene chains.
- IT **233756-39-3P**
(EQCM anal. of alkali metal ion coordination properties of
poly(thiophene)s 3,4-functionalized with crown-ether moieties)
- RN 233756-39-3 HCA
- CN Thieno[3,4-b]-1,4,7,10,13,16-hexaoxacyclooctadecin,
17,19-dibromo-2,3,5,6,8,9,11,12,14,15-decahydro- (9CI) (CA INDEX
NAME)



- IT Cyclic voltammetry
Electric conductivity

- (EQCM anal. of alkali metal ion coordination properties of poly(thiophene)s 3,4-functionalized with crown-ether moieties)
- IT Polymerization
(electrochem.; EQCM anal. of alkali metal ion coordination properties of poly(thiophene)s 3,4-functionalized with crown-ether moieties)
- IT 7439-93-2, Lithium, properties 7440-23-5, Sodium, properties
(EQCM anal. of alkali metal ion coordination properties of poly(thiophene)s 3,4-functionalized with crown-ether moieties)
- IT 249513-23-3P 484640-50-8P 484640-51-9P 497937-33-4P
497937-34-5P
(EQCM anal. of alkali metal ion coordination properties of poly(thiophene)s 3,4-functionalized with crown-ether moieties)
- IT 122372-75-2 126213-50-1 484640-48-4 484640-49-5
(EQCM anal. of alkali metal ion coordination properties of poly(thiophene)s 3,4-functionalized with crown-ether moieties)
- IT 233756-39-3P 497937-32-3P
(EQCM anal. of alkali metal ion coordination properties of poly(thiophene)s 3,4-functionalized with crown-ether moieties)

L27 ANSWER 11 OF 26 HCA COPYRIGHT 2005 ACS on STN

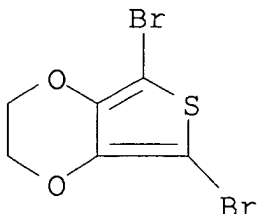
138:178716 Cyano-substituted oligothiophenes: a new approach to n-type organic semiconductors. Yassar, Abderrahim; Demanze, Frederic; Jaafari, Abdelhafid; El Idrissi, Mustapha; Coupry, Claude (ITODYS, Paris, F-75005, Fr.). Advanced Functional Materials, 12(10), 699-708 (English) 2002. CODEN: AFMDC6. ISSN: 1616-301X. Publisher: Wiley-VCH Verlag GmbH & Co. KGaA.

AB A series of α,ω -cyano oligothiophenes with three to six rings, as well as seven β,β' -substituted cyano terthiophenes have been synthesized using a palladium-catalyzed coupling reaction via organotin or organozinc intermediates. The structure of an oligothiophene trimer has been detd. by X-ray crystallog.; its space group is monoclinic (C2/c) with four mols. per unit cell ($Z = 4$). The mols. adopt the π - π stacking structure. UV-vis spectra of these materials as thin films show a bathochromic shift compared to unsubstituted oligothiophenes. These bathochromic shifts are interpreted in the light of charge transfer exciton. Cyano end-capped sexithiophene (CN-6T-CN) sandwiched between various metals (metal/CN-6T-CN/metal), to form Schottky diode structures, were fabricated by vapor deposition. The electron injection and rectification ratio strongly depend on the metal contact, namely the work function of the metal is compatible with the electron affinity of the org. material. The current-voltage results are compatible with n-type conduction in CN-6T-CN.

IT 174508-31-7
(prepn. of cyano-substituted oligothiophenes as n-type org. semiconductors)

RN 174508-31-7 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro- (9CI) (CA INDEX NAME)



- IT Exciton
(charge-transfer; prepn. of cyano-substituted oligothiophenes as n-type org. semiconductors)
- IT Coupling reaction
Crystal structure-property relationship
Electric current-potential relationship
Electron transport
Molecular structure-property relationship
NMR (nuclear magnetic resonance)
Schottky diodes
Semiconductor materials
UV and visible spectra
Work function
(prepn. of cyano-substituted oligothiophenes as n-type org. semiconductors)
- IT 1461-22-9D, Tributyltin chloride, derivs.
(Tributyltin; prepn. of cyano-substituted oligothiophenes as n-type org. semiconductors)
- IT 14221-01-3, Tetrakis(triphenylphosphine)palladium
(prepn. of cyano-substituted oligothiophenes as n-type org. semiconductors)
- IT 7429-90-5, Aluminum, uses 7440-22-4, Silver, uses 7440-57-5, Gold, uses
(prepn. of cyano-substituted oligothiophenes as n-type org. semiconductors)
- IT 110230-97-2P 134273-55-5P 176787-98-7P 176788-00-4P
183069-73-0P 188564-97-8P 188564-98-9P
(prepn. of cyano-substituted oligothiophenes as n-type org. semiconductors)
- IT 241495-53-4P
(prepn. of cyano-substituted oligothiophenes as n-type org. semiconductors)
- IT 109-72-8, reactions 544-92-3, Copper cyanide CuCN 1003-09-4, 2-Bromothiophene 1081-34-1, 2,2':5',2''-Terthiophene 1189-71-5, N-Chlorosulfonyl isocyanate 1641-09-4, 3-Cyanothiophene 3141-27-3, 2,5-Dibromothiophene 3480-11-3, 5-Bromo-2,2'-

bithiophene 4111-54-0, Lithium diisopropylamide 7646-85-7, Zinc chloride, reactions 18853-32-2, 3,4-Dicyanothiophene 94581-95-0, 5-Bromo-2,2':5',2''-terthiophene 98057-08-0 **174508-31-7** 176787-97-6 176787-99-8 497839-26-6 497839-27-7 497839-28-8 497839-29-9

(prepn. of cyano-substituted oligothiophenes as n-type org. semiconductors)

IT 2160-62-5P, 5-Bromo-2-cyanothiophene 145483-63-2P, 2,5-Bis(tributylstannyl)thiophene 171290-94-1P 176787-96-5P (prepn. of cyano-substituted oligothiophenes as n-type org. semiconductors)

L27 ANSWER 12 OF 26 HCA COPYRIGHT 2005 ACS on STN

136:200547 Neutral poly(3,4-ethylenedioxythiophene-2,5-diyl)s: preparation by organometallic polycondensation and their unique p-doping behavior. Yamamoto, Takakazu; Shiraishi, Kouichi; Abila, Mahmut; Yamaguchi, Isao; Groenendaal, L. "Bert" (Chemical Resources Laboratory, Tokyo Institute of Technology, Yokohama, Midori-ku, 226-8503, Japan). Polymer, Volume Date 2002, 43(3), 711-719 (English) 2001. CODEN: POLMAG. ISSN: 0032-3861. Publisher: Elsevier Science Ltd..

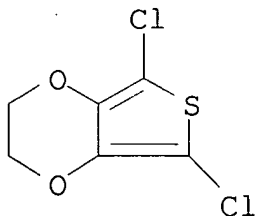
AB Neutral and non-doped poly(3,4-ethylenedioxythiophene), PEDOT_h(Ni), and its hexyl deriv., PEDOT_h-C₆(Ni), have been prepd. by organometallic dehalogenation polycondensation of 2,5-dichloro-3,4-ethylenedioxythiophene and its hexyl deriv. with a zerovalent nickel complex. PEDOT_h-C₆(Ni) was sol. in org. solvents and ¹H NMR data indicated that it had an Mn of 11,000. MALDI-TOF mass anal. of PEDOT_h(Ni) gave Mn and Mw of about 1700 and 2400, resp. PEDOT_h-C₆(Ni) showed a UV-Vis absorption peak at 546 nm in CHCl₃. Electrochem. oxidn. of PEDOT_h-C₆(Ni) started at about -0.40 V vs Ag⁺/Ag and gave a peak at 0.20 V vs Ag⁺/Ag. Chem. and electrochem. oxidn. (or p-doping) of PEDOT_h-C₆(Ni), both in solns. and in a solid state, led to weakening of the original π - π^* peaks and rise of new peak(s) in a region of 800-1500 nm. The p-doping of PEDOT_h-C₆(Ni) caused not only a decrease in the intensity of ¹H NMR signals of the bridging ethylene hydrogens but also a decrease in that of the hexyl side chain, suggesting a strong interaction of the p-dopant with the side chain. NMR data of poly(3-methoxythiophene-2,5-diyl) also supported an assumption that p-doping brings about a severe change in electronic state of the substituent attached to the polythiophene main chain. PEDOT_h(Ni) had a d. of 1.71 g cm⁻³; the mol. packing mode of PEDOT_h(Ni) is discussed based on the d. of the polymer and its XRD data.

IT **225518-49-0P 350827-42-8P**

(prepn. of neutral poly(ethylenedioxythiophenediyl)s by organometallic polycondensation and their unique p-doping behavior)

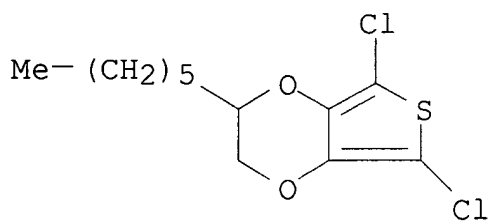
RN 225518-49-0 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dichloro-2,3-dihydro- (9CI) (CA INDEX NAME)



RN 350827-42-8 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dichloro-2-hexyl-2,3-dihydro- (9CI) (CA INDEX NAME)



IT Electric conductivity
(prepn. of neutral poly(ethylenedioxythiophenediyl)s by organometallic polycondensation and their unique p-doping behavior)

IT 163359-60-2P 225518-50-3P 350827-43-9P 351317-30-1P
(prepn. of neutral poly(ethylenedioxythiophenediyl)s by organometallic polycondensation and their unique p-doping behavior)

IT 126213-50-1 126213-53-4
(prepn. of neutral poly(ethylenedioxythiophenediyl)s by organometallic polycondensation and their unique p-doping behavior)

IT **225518-49-0P 350827-42-8P**
(prepn. of neutral poly(ethylenedioxythiophenediyl)s by organometallic polycondensation and their unique p-doping behavior)

L27 ANSWER 13 OF 26 HCA COPYRIGHT 2005 ACS on STN

135:242592 Optical and electrochemical properties of soluble N-hexylcarbazole-co-3,4-ethylenedioxythiophene copolymers. Beouch, L.; Tran Van, F.; Stephan, O.; Vial, J. C.; Chevrot, C. (Equipe Reactivite aux Interfaces (EA 2528), Laboratoire sur les Polymeres et les Materiaux Electroactifs, Universite de Cergy Pontoise, Cergy

Pontoise, 95013, Fr.). Synthetic Metals, 122(2), 351-358 (English) 2001. CODEN: SYMEDZ. ISSN: 0379-6779. Publisher: Elsevier Science S.A..

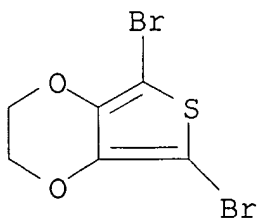
AB Sol. N-hexylcarbazole-co-3,4-ethylenedioxythiophene (HCz-co-EDOT) copolymers from mixts. in various ratio of the two corresponding dihalogenated monomers were synthesized. The random copolymers were obtained from EDOT/HCz starting molar ratio: 0.25, 1, 4, named, resp., C1, C2 and C3, and compared their properties to the two homopolymers synthesized in the same way. The IR studies clearly indicated, that an increase in the amt. of ethylenedioxythiophene in the feed compn. leads to an increase of the proportion of the corresponding comonomer in the final materials. Elemental anal. point out that the reactivity of dibrominated EDOT seems slightly lower than that of dibrominated HCz. Thin films of copolymer have been prepd. and their electrochem. response have been investigated. Absorption and luminescence of these materials have been also studied in CHCl₃. Copolymers mainly composed of one monomer (C1 and C3) behaves like the corresponding homopolymers. On an other hand, copolymer (C2) obtained from an equimolar amt. of each monomer in the feed compn. clearly exhibits distinct signals in optical spectra and in electrochem. behavior, probably due to the presence of each monomer unit short segments. The use of C2 has been explored for possible application in light emitting devices indicating that the p-doping of the material would be facilitated leading to an improved hole injecting when compared to carbazole homopolymer. It could be particularly interesting as a hole transporting layer in multilayer org. light emitting devices.

IT 174508-31-7P

(optical and electrochem. properties of sol. N-hexylcarbazole-co-3,4-ethylenedioxythiophene copolymers)

RN 174508-31-7 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro- (9CI) (CA INDEX NAME)



IT Absorption spectra
Cyclic voltammetry
Fluorescence
Hole transport
Luminescence

- Luminescence, electroluminescence
(optical and electrochem. properties of sol. N-hexylcarbazole-co-3,4-ethylenedioxythiophene copolymers)
- IT Band gap
(optical; optical and electrochem. properties of sol. N-hexylcarbazole-co-3,4-ethylenedioxythiophene copolymers)
- IT Polymers, preparation
(polythiophenes, carbazole group-contg.; optical and electrochem. properties of sol. N-hexylcarbazole-co-3,4-ethylenedioxythiophene copolymers)
- IT 7440-66-6, Zinc, uses
(activated; optical and electrochem. properties of sol. N-hexylcarbazole-co-3,4-ethylenedioxythiophene copolymers)
- IT 56-37-1, Triethylbenzylammonium chloride
(optical and electrochem. properties of sol. N-hexylcarbazole-co-3,4-ethylenedioxythiophene copolymers)
- IT 163359-60-2P 350037-71-7P 359829-15-5P 359829-16-6P 359829-17-7P, Poly(9-hexyl-9H-carbazole-3,6-diyl)
(optical and electrochem. properties of sol. N-hexylcarbazole-co-3,4-ethylenedioxythiophene copolymers)
- IT 111-25-1, Hexyl bromide 128-08-5, N-Bromosuccinimide 6825-20-3, 3,6-Dibromocarbazole 126213-50-1, 3,4-Ethylenedioxythiophene
(optical and electrochem. properties of sol. N-hexylcarbazole-co-3,4-ethylenedioxythiophene copolymers)
- IT 150623-72-6P 174508-31-7P
(optical and electrochem. properties of sol. N-hexylcarbazole-co-3,4-ethylenedioxythiophene copolymers)
- IT 46389-47-3, 2,2'-Bipyridinenickel dibromide
(polymn. catalyst; optical and electrochem. properties of sol. N-hexylcarbazole-co-3,4-ethylenedioxythiophene copolymers)

L27 ANSWER 14 OF 26 HCA COPYRIGHT 2005 ACS on STN

135:122840 Preparation of a soluble and neutral alkyl derivative of poly(3,4-ethylene-dioxythiophene) and its optical properties. Shiraishi, K.; Kanbara, T.; Yamamoto, T.; Groenendaal, L. B. (Chemical Resources Laboratory, Tokyo Institute of Technology, Nagatsuta, Midori-ku, Yokohama, 226-8503, Japan). Polymer, 42(16), 7229-7232 (English) 2001. CODEN: POLMAG. ISSN: 0032-3861. Publisher: Elsevier Science Ltd..

AB Sol. and non-doped poly(3,4-ethylenedioxythiophene) with a hexyl substituent (PEDOTh-C6 (Ni)), was first synthesized by Ni promoted dehalogenation polycondensation of the corresponding monomer. PEDOTh-C6 (Ni) exhibited good soly. in common org. solvents such as CHCl₃, CH₂Cl₂, and DMF, in contrast to poor soly. of the corresponding polymer synthesized by oxidative polymn. GPC anal. indicated that PEDOTh-C6 (Ni) had Mn and Mw of 5400 and 8500 (vs polystyrene stds.); ¹H NMR anal. gave an Mn value of 11,000. A cast film of PEDOTh-C6 (Ni) received electrochem. p-doping at 0.20 V vs

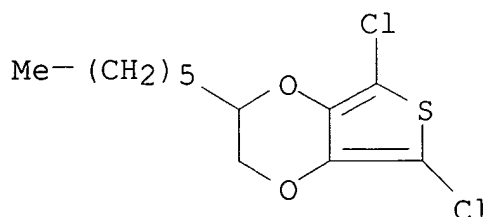
Ag+/Ag. Chem. and electrochem. oxidn. of PEDOT_h-C6 (Ni) led to appearance of new absorption bands in the near IR region.

IT 350827-42-8P

(monomer; prepn. of a sol. and neutral hexyl deriv. of poly(3,4-ethylene-dioxythiophene) and optical properties of nondoped and doped polymers)

RN 350827-42-8 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dichloro-2-hexyl-2,3-dihydro- (9CI)
(CA INDEX NAME)



IT Dopants

Doping

UV and visible spectra

(prepn. of a sol. and neutral hexyl deriv. of poly(3,4-ethylene-dioxythiophene) and optical properties of nondoped and doped polymers)

IT 7553-56-2, Iodine, uses

(dopant; prepn. of a sol. and neutral hexyl deriv. of poly(3,4-ethylene-dioxythiophene) and optical properties of nondoped and doped polymers)

IT 350827-42-8P

(monomer; prepn. of a sol. and neutral hexyl deriv. of poly(3,4-ethylene-dioxythiophene) and optical properties of nondoped and doped polymers)

IT 1295-35-8, Bis(1,5-cyclooctadiene)nickel

(polymn. catalyst; prepn. of a sol. and neutral hexyl deriv. of poly(3,4-ethylene-dioxythiophene) and optical properties of nondoped and doped polymers)

IT 350827-43-9P 351317-30-1P

(prepn. of a sol. and neutral hexyl deriv. of poly(3,4-ethylene-dioxythiophene) and optical properties of nondoped and doped polymers)

IT 128-09-6, N-Chlorosuccinimide

(reactant in monomer prepn.; prepn. of a sol. and neutral hexyl deriv. of poly(3,4-ethylene-dioxythiophene) and optical properties of nondoped and doped polymers)

L27 ANSWER 15 OF 26 HCA COPYRIGHT 2005 ACS on STN

135:107664 Fully undoped and soluble oligo(3,4-ethylenedioxythiophene)s:

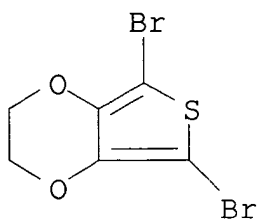
spectroscopic study and electrochemical characterization. Tran-Van, Francois; Garreau, Sebastien; Louarn, Guy; Froyer, Gerard; Chevrot, Claude (Equipe Reactivite aux Interfaces (EA 2528), Laboratoire sur les Polymeres et les Materiaux Electroactifs, Universite de Cergy Pontoise, Cergy Pontoise, 95013, Fr.). Journal of Materials Chemistry, 11(5), 1378-1382 (English) 2001. CODEN: JMACEP. ISSN: 0959-9428. Publisher: Royal Society of Chemistry.

AB Fully undoped oligo(3,4-ethylenedioxythiophene)s were synthesized via polycondensation of the dibromo monomer in the presence of NiBr₂(bpy) catalyst in N,N-dimethylacetamide (DMA). HPLC anal. indicated that the material is constituted of three main oligomers which were clearly detected by UV-Visible spectroscopy. The polythiophenes are partially sol. in DMA making them easier to process to produce thin films of oligomers by evapn. of the solvent. Electrochem. and electrochromic properties of undoped films were studied. Deep purple in its undoped state, the material becomes sky blue in the oxidized form. The mixt. of oligomers was characterized by Raman scattering, IR absorption and X-Ray diffraction, and compared to poly(3,4-ethylenedioxy thiophene) obtained by the oxidative route.

IT 174508-31-7P, 2,5-Dibromo-3,4-ethylenedioxythiophene
(monomer; prepn. and redox electrochem. of electroactive fully undoped and sol. oligo(3,4-ethylenedioxythiophene)s)

RN 174508-31-7 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro- (9CI) (CA INDEX NAME)



IT Polymers, preparation
(conjugated; prepn. and redox electrochem. of electroactive fully undoped and sol. oligo(3,4-ethylenedioxythiophene)s)

IT Polymerization
(dehalogenation condensation; prepn. and redox electrochem. of electroactive fully undoped and sol. oligo(3,4-ethylenedioxythiophene)s)

IT Redox reaction
(electrochem.; prepn. and redox electrochem. of electroactive fully undoped and sol. oligo(3,4-ethylenedioxythiophene)s)

IT Polymer chains
(length, conjugation, low homogeneity; prepn. and redox

- electrochem. of electroactive fully undoped and sol.
oligo(3,4-ethylenedioxythiophene)s)
- IT Polymers, preparation
(polythiophenes, ethylenedioxythiophene, oligomeric; prepn. and
redox electrochem. of electroactive fully undoped and sol.
oligo(3,4-ethylenedioxythiophene)s)
- IT Conducting polymers
(polythiophenes; prepn. and redox electrochem. of electroactive
fully undoped and sol. oligo(3,4-ethylenedioxythiophene)s)
- IT Conjugation (bond)
Electrochromic materials
Electrochromism
Raman spectra
Redox potential
(prepn. and redox electrochem. of electroactive fully undoped and
sol. oligo(3,4-ethylenedioxythiophene)s)
- IT Band gap
(semiconductor; prepn. and redox electrochem. of electroactive
fully undoped and sol. oligo(3,4-ethylenedioxythiophene)s)
- IT 182628-58-6, (2,2'-Bipyridine)dibromonickel
(condensation polymn. catalyst; prepn. and redox electrochem. of
electroactive fully undoped and sol. oligo(3,4-
ethylenedioxythiophene)s)
- IT **174508-31-7P**, 2,5-Dibromo-3,4-ethylenedioxythiophene
(monomer; prepn. and redox electrochem. of electroactive fully
undoped and sol. oligo(3,4-ethylenedioxythiophene)s)
- IT 163359-60-2P 350037-71-7P
(oligomeric; prepn. and redox electrochem. of electroactive fully
undoped and sol. oligo(3,4-ethylenedioxythiophene)s)
- IT 128-08-5, N-Bromosuccinimide 126213-50-1, 3,4-
Ethylenedioxythiophene
(prepn. and redox electrochem. of electroactive fully undoped and
sol. oligo(3,4-ethylenedioxythiophene)s)
- IT 127-19-5, N,N-Dimethylacetamide
(solvent; prepn. and redox electrochem. of electroactive fully
undoped and sol. oligo(3,4-ethylenedioxythiophene)s)

L27 ANSWER 16 OF 26 HCA COPYRIGHT 2005 ACS on STN

134:287964 Organic compound for organic electroluminescence member.
Hosokawa, Chishio; Ikeda, Shuji (Idemitsu Kosan Co., Ltd., Japan).
Jpn. Kokai Tokkyo Koho JP 2001097949 A2 20010410, 28 pp.
(Japanese). CODEN: JKXXAF. APPLICATION: JP 1999-277956 19990930.

AB The title org. compd. is represented by
[Ar4Ar5C=CR1]s{(Ar2)m(Ar1)k(Ar3)n}w[R2C=CAr6Ar7]t (Ar1 = divalent
org. group; Ar2,3 = C6-30 arylene, etc.; Ar4-7 = C6-20 aryl, etc.;
R1,2 = H, C1-6 alkyl, etc.; m, n, s, and t = 0, 1, 2). When the
org. compd. is used as a recombination site-forming substance and a
light-emitting material, the electroluminescence member gives high

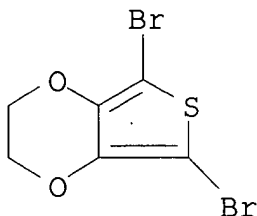
efficiency and long lifetime.

IT 174508-31-7

(org. compd. for org. electroluminescence member)

RN 174508-31-7 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro- (9CI) (CA INDEX NAME)



IT Electroluminescent devices

(org. compd. for)

IT 333432-12-5P 333432-14-7P 333432-16-9P 333432-18-1P
333432-20-5P 333432-22-7P 333432-24-9P

(org. compd. for org. electroluminescence member)

IT 15155-41-6 174508-31-7 201802-67-7 288105-04-4
333432-27-2 333432-28-3 333432-31-8

(org. compd. for org. electroluminescence member)

L27 ANSWER 17 OF 26 HCA COPYRIGHT 2005 ACS on STN

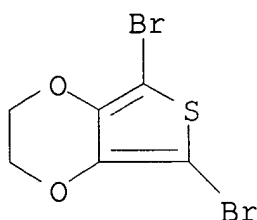
134:17569 Charge Transfer and Delocalization in Conjugated

(Ferrocenylethynyl)oligothiophene Complexes. Zhu, Yongbao; Wolf, Michael O. (Department of Chemistry, University of British Columbia, Vancouver, BC, V6T 1Z1, Can.). Journal of the American Chemical Society, 122(41), 10121-10125 (English) 2000. CODEN: JACSAT. ISSN: 0002-7863. OTHER SOURCES: CASREACT 134:17569. Publisher: American Chemical Society.

AB Conjugated mono(ferrocenylethynyl)oligothiophene and bis(ferrocenylethynyl)oligothiophene complexes were prepd. The cyclic voltammograms of the complexes all contain a reversible ferrocene oxidn. wave and an irreversible oligothiophene-based wave. The p.d. between the two waves (ΔE) varies from 0.38 to 1.12 V, depending on the length and substitution of the oligothiophene group. Several of the mono(ferrocenylethynyl)oligothiophene complexes couple when oxidized, resulting in the deposition of a redox-active film on the electrode surface. In soln., electrochem. oxidn. of the FeII centers yields the corresponding monocations and dications, which exhibit oligothiophene-to-FeIII charge-transfer transitions in the near-IR region. The band maxima of these low-energy transitions correlate linearly with ΔE , while the oscillator strengths show a linear correlation with neg. slope with ΔE . The complexes with similar charge-transfer transition

dipole lengths show an increase in the extent of charge delocalization with smaller ΔE . Comparisons between complexes with different length oligothiophene ligands show that a redn. in ΔE results either in greater delocalization of charge or in charge being delocalized further along the rigid oligothiophene ligand. These results have important implications in understanding charge delocalization in metal-contg. polymers.

IT 174508-31-7P, 2,5-Dibromo-3,4-ethylenedioxythiophene
(prepn., coupling with bromothiophene and conversion to monobromo analog)
RN 174508-31-7 HCA
CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro- (9CI) (CA INDEX NAME)



IT Charge transfer transition
(LMCT; of conjugated mono(ferrocenylethynyl)oligothiophene and bis(ferrocenylethynyl)oligothiophene complexes)
IT Redox reaction
(electrochem.; of mono(ferrocenylethynyl)oligothiophene and bis(ferrocenylethynyl)oligothiophene complexes)
IT Films
(electrochromic; formation on electrode surface of redox-active films from mono(ferrocenylethynyl)oligothiophene complexes when electrochem. oxidized)
IT Metallocenes
(ferrocenes; prepn., cyclic voltammetry, LMCT transitions and delocalization in mono(ferrocenylethynyl)oligothiophene and bis(ferrocenylethynyl)oligothiophene complexes)
IT Electrochromic materials
(films; formation on electrode surface of redox-active films from mono(ferrocenylethynyl)oligothiophene complexes when electrochem. oxidized)
IT Electron delocalization
(in conjugated mono(ferrocenylethynyl)oligothiophene and bis(ferrocenylethynyl)oligothiophene complexes)
IT Linear free energy relationship
(of LMCT transitions and oscillator strengths of mono(ferrocenylethynyl)oligothiophene and bis(ferrocenylethynyl)oligothiophene complexes with p.d. between

- ferrocene oxidn. and oligothiophene-based waves)
- IT Oxidation, electrochemical
Oxidation potential
Redox potential
(of mono(ferrocenylethynyl)oligothiophene and
bis(ferrocenylethynyl)oligothiophene complexes)
- IT Oscillator strength
(of mono(ferrocenylethynyl)oligothiophene and
bis(ferrocenylethynyl)oligothiophene complexes in relation to
p.d. between ferrocene oxidn. and oligothiophene-based waves)
- IT Coupling reaction
(of mono(ferrocenylethynyl)oligothiophene complexes when
electrochem. oxidized)
- IT 126213-50-1, 3,4-Ethylenedioxythiophene
(bromination of)
- IT 1003-09-4, 2-Bromothiophene
(coupling reactions with dibromoethylenedioxythiophene and
ethynylferrocene)
- IT 1271-47-2, Ethynylferrocene
(coupling reactions with halo-substituted thiophene oligomers)
- IT 3141-27-3, 2,5-Dibromothiophene 3480-11-3, 5-Bromo-2,2'-
bithiophene 4805-22-5, 5,5'-DiBromo-2,2'-bithiophene 98057-08-0,
5,5''-Dibromo-2,2':5',2''-terthiophene 104499-98-1,
5-Iodo-2,2':5',2''-terthiophene
(coupling with ethynylferrocene)
- IT 309753-41-1 309753-42-2 309753-43-3 309753-44-4 309753-45-5
309753-46-6 309753-47-7 309753-48-8 309753-49-9 309753-50-2
(electrochem. formation, UV-visible-near-IR spectra and elec.
potential of couple contg.)
- IT 309753-55-7P 309753-58-0P 309753-60-4P
(electrochromic films)
- IT 309753-52-4P, 3',4'-Ethylenedioxy-2,2':5',2''-terthiophene
(prepn. and bromination of)
- IT 302554-82-1P, 2-Bromo-3,4-ethylenedioxythiophene 309753-53-5P,
5-Bromo-3',4'-ethylenedioxy-2,2':5',2''-terthiophene 309753-54-6P,
5,5''-Dibromo-3',4'-ethylenedioxy-2,2':5',2''-terthiophene
(prepn. and coupling with ethynylferrocene)
- IT 174508-31-7P, 2,5-Dibromo-3,4-ethylenedioxythiophene
(prepn., coupling with bromothiophene and conversion to monobromo
analog)
- IT 1291-88-9P, 2-Ferrocenylethynylthiophene 261622-36-0P,
2,5-Bis(ferrocenylethynyl)thiophene 261622-40-6P,
5,5'-Bis(ferrocenylethynyl)-2,2'-bithiophene 261622-46-2P,
5,5''-Bis(ferrocenylethynyl)-2,2':5',2''-terthiophene
309753-33-1P, 5-Ferrocenylethynyl-2,2'-bithiophene 309753-35-3P,
5-Ferrocenylethynyl-2,2':5',2''-terthiophene 309753-36-4P,
5-Ferrocenylethynyl-3,4-ethylenedioxythiophene 309753-37-5P,
5-Ferrocenylethynyl-3',4'-ethylenedioxy-2,2':5',2''-terthiophene

309753-39-7P, 2,5-Bis(ferrocenylethynyl)-3,4-ethylenedioxythiophene
309753-40-0P, 5,5''-Bis(ferrocenylethynyl)-3',4'-ethylenedioxy-
2,2':5',2''-terthiophene

(prepn., cyclic voltammetry, LMCT transitions and delocalization
in mono(ferrocenylethynyl)oligothiophene and
bis(ferrocenylethynyl)oligothiophene complexes)

L27 ANSWER 18 OF 26 HCA COPYRIGHT 2005 ACS on STN

133:223287 Synthesis and Electronic Structure Investigations of
 α,ω -Bis(arylthio)oligothiophenes: Toward Understanding
Wire-Linker Interactions in Molecular-Scale Electronic Materials.
Hicks, Robin G.; Nodwell, Matthew B. (Department of Chemistry,
University of Victoria, Victoria, BC, V8W 3V6, Can.). Journal of
the American Chemical Society, 122(28), 6746-6753 (English) 2000.
CODEN: JACSAT. ISSN: 0002-7863. Publisher: American Chemical
Society.

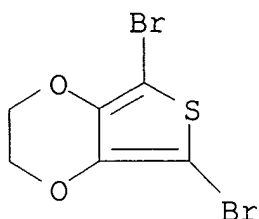
AB Several oligothiophenes with 2-mesitylthio (MesS) substituents have
been prepd. and studied by UV-visible spectroscopy and cyclic
voltammetry. These compds. can be considered as models for
thiol-terminated conjugated oligomers, which have attracted intense
interest as materials for mol.-scale electronics. Three types of
oligomers were prepd.: α,ω -bis(mesitylthio)oligothiophen
es 4-7, α,ω -bis(mesitylthio)oligo(3,4-
ethylelendioxythiophene)s 12-14, and α,ω -
bis(mesitylthio)oligomers 15-19 contg. both thiophene and
3,4-ethylenedioxythiophene rings. The mesitylthio groups were
introduced via nucleophilic attack of lithiated thiophenes on
mesitylenesulfenyl chloride. The oligomers were assembled by
oxidative coupling or palladium-catalyzed Stille coupling of
2-stannylthiophenes with 2-bromothiophenes. The soln. electronic
spectra of all oligomers display a red-shift in the lowest-energy
transition max. (λ_{max}) relative to oligothiophenes lacking
the MesS- group. The red-shift arises from conjugative overlap of a
mesitylthio sulfur lone pair with the oligothiophene π system.
Cyclic voltammetry studies indicate that the MesS group
significantly lowers the first and second oxidn. potentials of the
oligomers and improves the stability of the incipient radical
cations and dications relative to alkyl-capped oligothiophenes.
Addnl., the difference between first and second oxidn. potentials in
the MesS-substituted oligomers is much lower than known
alkyl-substituted oligomers. This effect is due to the terminal
MesS groups which cause charge d. in the radical cations to conc. at
the chain ends, thereby lowering the Coulombic barrier to
introduction of a second charge. The electronic structure
perturbations caused by the MesS- group are discussed in the context
of single-mol. conduction in thiol-terminated conjugated oligomers
bound to gold electrodes.

IT 174508-31-7P, 2,5-Dibromo-3,4-ethylenedioxythiophene

(synthesis and electronic structure of α,ω -bis(arylthio)oligothiophenes)

RN 174508-31-7 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro- (9CI) (CA INDEX NAME)



IT Oxidation potential

(first, second; synthesis and electronic structure of α,ω -bis(arylthio)oligothiophenes)

IT Conducting polymers

Cyclic voltammetry

(synthesis and electronic structure of α,ω -bis(arylthio)oligothiophenes)

IT 291308-71-9P 291308-72-0P 291308-73-1P 291308-74-2P
291308-77-5P 291308-78-6P 291308-79-7P 291308-80-0P
291308-81-1P 291308-82-2P 291308-83-3P 291308-85-5P

(synthesis and electronic structure of α,ω -bis(arylthio)oligothiophenes)

IT 1541-10-2, Mesitylenethiol 3141-27-3, 2,5-Dibromothiophene

(synthesis and electronic structure of α,ω -bis(arylthio)oligothiophenes)

IT 14575-12-3P, 2-Mesitylenesulphenyl chloride 174508-31-7P,
2,5-Dibromo-3,4-ethylenedioxythiophene 291308-70-8P 291308-75-3P
291308-76-4P

(synthesis and electronic structure of α,ω -bis(arylthio)oligothiophenes)

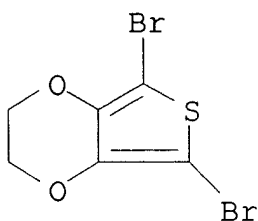
L27 ANSWER 19 OF 26 HCA COPYRIGHT 2005 ACS on STN

133:208463 Molecular Design and Characterization of Chromic Polyfluorene Derivatives. Blondin, Pierre; Bouchard, Jimmy; Beaupre, Serge; Belletete, Michel; Durocher, Gilles; Leclerc, Mario (Departement de Chimie Centre de Recherche en Sciences et Ingenierie des Macromolecules, Universite Laval, Quebec, QC, G1K 7P4, Can.). Macromolecules, 33(16), 5874-5879 (English) 2000. CODEN: MAMOBX. ISSN: 0024-9297. Publisher: American Chemical Society.

AB The thermochromic and solvatochromic properties of a series of fluorene-based conjugated polymers have been investigated. Both poly(2,7-(9,9-dioctylfluorene)) and poly(2,5-(thiophene)-alt-2,7-(9,9-dioctylfluorene)) have revealed interesting chromic properties

which, on the basis of theor. calcns., seem to be related to a relatively flexible backbone. On the other hand, the sterically hindered, nonplanar poly(2,5-(3,4-dimethylthiophene)-alt-2,7-(9,9-dioctylfluorene)) does not exhibit any significant solvatochromic and thermochromic properties which could be explained by an important energy barrier against planarity. Finally, investigations on poly(2,5-(3,4-ethylenedioxythiophene)-alt-2,7-(9,9-dioctylfluorene)) have revealed a highly conjugated conformational structure which is not significantly modified upon temp. or solvent changes.

IT **174508-31-7P**, 2,5-Dibromo-3,4-ethylenedioxythiophene
(mol. design and characterization of chromic polyfluorene
derivs.)
RN 174508-31-7 HCA
CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro- (9CI) (CA INDEX
NAME)



IT Polymers, properties
(fluorene-based; mol. design and characterization of chromic
polyfluorene derivs.)
IT Potential barrier
Potential energy
Solvatochromism
Thermochromism
UV and visible spectra
(mol. design and characterization of chromic polyfluorene
derivs.)
IT Bond angle
(torsional; mol. design and characterization of chromic
polyfluorene derivs.)
IT 123864-00-6, Poly(9,9-dioctylfluorene) 222857-60-5 222857-62-7
287924-57-6 287924-58-7 287924-59-8 287924-60-1
(mol. design and characterization of chromic polyfluorene
derivs.)
IT 3141-26-2, 3,4-Dibromothiophene
(mol. design and characterization of chromic polyfluorene
derivs.)
IT 74707-05-4P, 2,5-Dibromo-3,4-dimethylthiophene **174508-31-7P**
, 2,5-Dibromo-3,4-ethylenedioxythiophene

(mol. design and characterization of chromic polyfluorene derivs.)

L27 ANSWER 20 OF 26 HCA COPYRIGHT 2005 ACS on STN

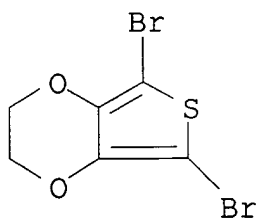
133:164431 Light-Emitting Diodes from Fluorene-Based π -Conjugated Polymers. Donat-Bouillud, Anne; Levesque, Isabelle; Tao, Ye; D'Iorio, Marie; Beaupre, Serge; Blondin, Pierre; Ranger, Maxime; Bouchard, Jimmy; Leclerc, Mario (Institute for Microstructural Sciences, National Research Council of Canada, Ottawa, ON, K1A 0R6, Can.). Chemistry of Materials, 12(7), 1931-1936 (English) 2000. CODEN: CMATEX. ISSN: 0897-4756. Publisher: American Chemical Society.

AB The synthesis of fluorene-based π -conjugated polymers was carried out and the electroluminescent properties of the polymers were studied. The photo- and electroluminescence of poly(dioctylfluorene-phenylene)s and poly(dioctylfluorene-thiophene)s whose synthesis was recently published was also studied. The alternate incorporation of phenylene or thiophene moieties in fluorene-based π -conjugated polymers was used to effect tunability of electroluminescent properties. The spectral emission varies from blue to green or yellow, depending on the compn. of the copolymers. To enhance the luminescence efficiency of polymer assemblies, hole injection and hole transport into the polymer were improved by insertion of an insulating buffer layer and the incorporation of efficient hole transport material in the polymer. The insertion of a charge injection layer such as LiF and a hole transport layer such as N,N'-diphenyl-N,N'-bis(3-methylphenyl)-1,1-biphenyl-4,4'-diamine significantly improved the electroluminescence efficiency of a test diode from 4.5 to 125 cd/m².

IT 174508-31-7P, 2,5-Dibromo-3,4-ethylenedioxythiophene (monomer; prepn. of poly(dioctylfluorene-thiophene)s with tunable electroluminescence and improved carrier transport for use in light-emitting diodes)

RN 174508-31-7 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro- (9CI) (CA INDEX NAME)



IT Polymerization (Suzuki coupling; prepn. of poly(dioctylfluorene-thiophene)s with

- tunable electroluminescence and improved carrier transport for use in light-emitting diodes)
- IT Polymers, preparation
(conjugated; prepn. of poly(dioctylfluorene-thiophene)s with tunable electroluminescence and improved carrier transport for use in light-emitting diodes)
- IT Electroluminescent devices
(light emitting diodes; prepn. of poly(dioctylfluorene-thiophene)s with tunable electroluminescence and improved carrier transport for use in light-emitting diodes)
- IT Polymers, preparation
(polythiophenes, polyfluorene; prepn. of poly(dioctylfluorene-thiophene)s with tunable electroluminescence and improved carrier transport for use in light-emitting diodes)
- IT Conducting polymers
Electrochromism
Hole transport
Luminescence, electroluminescence
Oxidation potential
Reduction potential
Suzuki coupling reaction
(prepn. of poly(dioctylfluorene-thiophene)s with tunable electroluminescence and improved carrier transport for use in light-emitting diodes)
- IT Electric current carriers
(transport; prepn. of poly(dioctylfluorene-thiophene)s with tunable electroluminescence and improved carrier transport for use in light-emitting diodes)
- IT 7789-24-4, Lithium fluoride (LiF), properties
(carrier injection layer; prepn. of poly(dioctylfluorene-thiophene)s with tunable electroluminescence and improved carrier transport for use in light-emitting diodes)
- IT 65181-78-4, N,N'-Diphenyl-N,N'-bis(3-methylphenyl)-1,1-biphenyl-4,4'-diamine
(hole transport layer; prepn. of poly(dioctylfluorene-thiophene)s with tunable electroluminescence and improved carrier transport for use in light-emitting diodes)
- IT 195602-17-6P, 2,2'-Bis(3,4-ethylenedioxy)bithiophene
(monomer and intermediate; prepn. of poly(dioctylfluorene-thiophene)s with tunable electroluminescence and improved carrier transport for use in light-emitting diodes)
- IT 74707-05-4P, 2,5-Dibromo-3,4-dimethylthiophene 174508-31-7P
, 2,5-Dibromo-3,4-ethylenedioxythiophene 287924-56-5P
(monomer; prepn. of poly(dioctylfluorene-thiophene)s with tunable electroluminescence and improved carrier transport for use in light-emitting diodes)
- IT 7440-05-3, Palladium, uses
(polymn. catalyst; prepn. of poly(dioctylfluorene-thiophene)s

with tunable electroluminescence and improved carrier transport for use in light-emitting diodes)

IT 198964-57-7P 198964-62-4P 210347-56-1P 222857-60-5P
222857-62-7P 222857-64-9P 222857-68-3P 222857-69-4P
287924-57-6P 287924-58-7P 287924-59-8P 287924-60-1P
287924-61-2P 287924-62-3P

(prepn. of poly(dioctylfluorene-thiophene)s with tunable electroluminescence and improved carrier transport for use in light-emitting diodes)

IT 75-16-1, Methylmagnesium bromide 128-08-5, NBS 3141-26-2,
3,4-Dibromothiophene 126213-50-1, 3,4-Ethylenedioxythiophene
(prepn. of poly(dioctylfluorene-thiophene)s with tunable electroluminescence and improved carrier transport for use in light-emitting diodes)

L27 ANSWER 21 OF 26 HCA COPYRIGHT 2005 ACS on STN

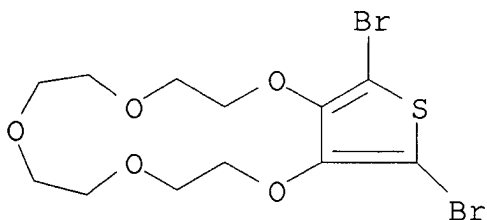
131:138509 Molecular recognition properties of crown ether-functionalized oligothiophenes. Rimmel, G.; Bauerle, P. (Abteilung Organische Chemie II, Universitat Ulm, Ulm, 89081, Germany). Synthetic Metals, 102(1-3), 1323-1324 (English) 1999. CODEN: SYMEDZ. ISSN: 0379-6779. Publisher: Elsevier Science S.A..

AB The palladium-catalyzed cross-coupling of dibrominated thieno-crown ethers and stannylated cyclohexyl-capped mono- or bithiophenes leads to novel end-capped oligothiophenes functionalized with crown ether units of different ring size which are directly linked to the oligomeric π -system. The electrochem. properties of these oligomers were studied in the presence of metal cations. Their redox chem. is strongly influenced by the mol. recognition process and by the polarity of the solvent system. Due to electrostatic interactions between the complexed cation and the redox center, the oxidn. of the oligothiophene π -system becomes more difficult leading to an anodic shift of the oxidn. potential.

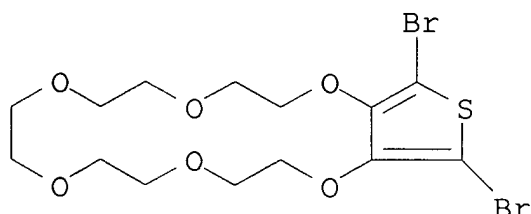
IT 163657-74-7 233756-39-3 233756-41-7
(prepn. and mol. recognition properties of crown ether-functionalized oligothiophenes)

RN 163657-74-7 HCA

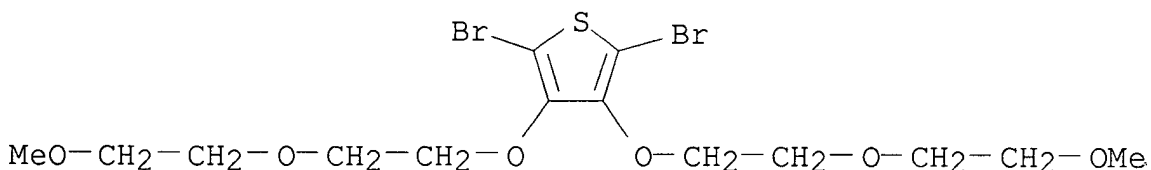
CN Thieno[3,4-b]-1,4,7,10,13-pentaoxacyclopentadecin,
14,16-dibromo-2,3,5,6,8,9,11,12-octahydro- (9CI) (CA INDEX NAME)



RN 233756-39-3 HCA
 CN Thieno[3,4-b]-1,4,7,10,13,16-hexaoxacyclooctadecin,
 17,19-dibromo-2,3,5,6,8,9,11,12,14,15-decahydro- (9CI) (CA INDEX
 NAME)

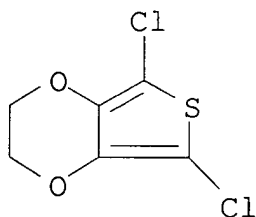


RN 233756-41-7 HCA
 CN Thiophene, 2,5-dibromo-3,4-bis[2-(2-methoxyethoxy)ethoxy]- (9CI)
 (CA INDEX NAME)



IT Alkali metals, analysis
 (ions; prepn. and mol. recognition properties of crown
 ether-functionalized oligothiophenes)
 IT Molecular recognition
 (prepn. and mol. recognition properties of crown
 ether-functionalized oligothiophenes)
 IT Crown ethers
 (prepn. and mol. recognition properties of crown
 ether-functionalized oligothiophenes)
 IT 7439-93-2, Lithium, analysis 7440-09-7, Potassium, analysis
 7440-23-5, Sodium, analysis 7440-39-3, Barium, analysis
 14798-03-9, Ammonium, analysis
 (prepn. and mol. recognition properties of crown
 ether-functionalized oligothiophenes)
 IT 233756-27-9P 233756-29-1P 233756-30-4P 233756-32-6P
 233756-34-8P 233756-36-0P
 (prepn. and mol. recognition properties of crown
 ether-functionalized oligothiophenes)
 IT 163657-74-7 218606-46-3 233756-37-1 233756-39-3
 233756-41-7
 (prepn. and mol. recognition properties of crown
 ether-functionalized oligothiophenes)

- L27 ANSWER 22 OF 26 HCA COPYRIGHT 2005 ACS on STN
131:74044 Synthesis of non-doped poly(3,4-ethylenedioxythiophene) and its spectroscopic data. Yamamoto, Takakazu; Abia, Mahmut (Research Laboratory of Resources Utilization, Tokyo Institute of Technology, Yokohama, Japan). Synthetic Metals, 100(2), 237-239 (English) 1999. CODEN: SYMEDZ. ISSN: 0379-6779. Publisher: Elsevier Science S.A..
- AB Non-doped poly(3,4-ethylenedioxythiophene) (PEDOT) has been synthesized by Ni-promoted dehalogenation polymn. of the corresponding 2,5-dichloro monomer. Its IR, NMR, and XRD data are compared with those of PEDOT prepd. by chem. oxidn. polymn.
- IT **225518-49-0P**, 2,5-Dichloro-3,4-ethylenedioxythiophene (prepn. and polycondensation of dichloroethylenedioxythiophene monomer)
- RN 225518-49-0 HCA
- CN Thieno[3,4-b]-1,4-dioxin, 5,7-dichloro-2,3-dihydro- (9CI) (CA INDEX NAME)



- IT Polymerization catalysts (nickel complex; for polycondensation of dichloroethylenedioxythiophene monomer)
- IT 1295-35-8, Bis(1,5-cyclooctadiene)nickel (catalyst for polycondensation of dichloroethylenedioxythiophene)
- IT 126213-50-1, 3,4-Ethylenedioxythiophene (chlorination; prepn. of dichloroethylenedioxythiophene monomer)
- IT 111-78-4, 1,5-Cyclooctadiene 366-18-7, 2,2'-Bipyridyl (in catalyst for polycondensation of dichloroethylenedioxythiophene)
- IT **225518-49-0P**, 2,5-Dichloro-3,4-ethylenedioxythiophene (prepn. and polycondensation of dichloroethylenedioxythiophene monomer)
- IT 225518-50-3P, 2,5-Dichloro-3,4-ethylenedioxythiophene homopolymer (prepn. of undoped polymer by polycondensation)
- IT 163359-60-2P, Poly(3,4-ethylenedioxythiophene-2,5-diyl) (prepn. of undoped polymer by polycondensation of dichloro monomer)

- L27 ANSWER 23 OF 26 HCA COPYRIGHT 2005 ACS on STN
124:203512 Absorption Properties of Alkoxy-Substituted Thienylene-Vinylene Oligomers as a Function of the Doping Level.

Havinga, E. E.; Mutsaers, C. M. J.; Jenneskens, L. W. (Philips Research Laboratories, Eindhoven, 5656 AA, Neth.). Chemistry of Materials, 8(3), 769-76 (English) 1996. CODEN: CMATEX. ISSN: 0897-4756. Publisher: American Chemical Society.

AB In an attempt to improve on the properties of PEDOT (poly(3,4-ethylenedioxythiophene)) as a stable, conducting, and transparent coating we synthesized four different alkoxy-substituted poly(thienylene-vinylene)s, 1-4, using the Stille coupling reaction. The oligomers and polymers obtained were characterized and their NIR-vis absorption spectra were measured as a function of doping, both electrochem. as films and chem. in soln. Similar spectra of PEDOT films were gathered for comparison. In PEDOT a change in doping level does not change the energies of the absorption bands, while for the other polymers the bands shift markedly and the NIR peak at high doping level lies at a higher energy. The polymers 1-4 are much less suited for the intended coatings than PEDOT. Possible reasons for this are discussed.

IT 173291-48-0P, 2,5-Dibromo-3,4-bis(dodecyloxy)thiophene

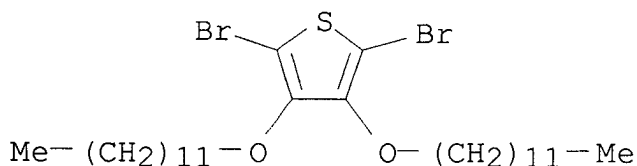
173291-49-1P, 2,5-Dibromo-3,4-dibutoxythiophene

173291-50-4P

(monomer; absorption properties of alkoxy-substituted thienylene-vinylene oligomers as a function of the doping level)

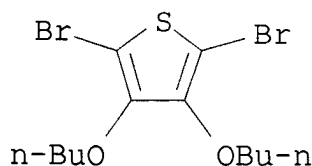
RN 173291-48-0 HCA

CN Thiophene, 2,5-dibromo-3,4-bis(dodecyloxy)- (9CI) (CA INDEX NAME)



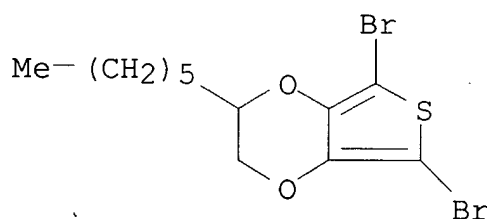
RN 173291-49-1 HCA

CN Thiophene, 2,5-dibromo-3,4-dibutoxy- (9CI) (CA INDEX NAME)



RN 173291-50-4 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2-hexyl-2,3-dihydro- (9CI)
(CA INDEX NAME)



- IT Electric conductivity and conduction
Electric conductors, polymeric
Oscillator strength
Ultraviolet and visible spectra
(absorption properties of alkoxy-substituted thienylene-vinylene oligomers as a function of the doping level)
- IT Infrared spectra
(near-; absorption properties of alkoxy-substituted thienylene-vinylene oligomers as a function of the doping level)
- IT Coating materials
(elec. conductive, transparent, absorption properties of alkoxy-substituted thienylene-vinylene oligomers as a function of the doping level)
- IT Energy level, band structure
(gap, absorption properties of alkoxy-substituted thienylene-vinylene oligomers as a function of the doping level)
- IT Electric potential
(oxidn., absorption properties of alkoxy-substituted thienylene-vinylene oligomers as a function of the doping level)
- IT Polymers, properties
(polythiophenes, -vinylenes; absorption properties of alkoxy-substituted thienylene-vinylene oligomers as a function of the doping level)
- IT 126213-54-5P 173291-56-0P 174592-79-1P
(absorption properties of alkoxy-substituted thienylene-vinylene oligomers as a function of the doping level)
- IT 126213-51-2, Poly(3,4-ethylenedioxythiophene)
(absorption properties of alkoxy-substituted thienylene-vinylene oligomers as a function of the doping level)
- IT 994-89-8P, Tributylethynyltin
(absorption properties of alkoxy-substituted thienylene-vinylene oligomers as a function of the doping level)
- IT 84-58-2, 2,3-Dicyano-5,6-dichloro-1,4-benzoquinone 7705-08-0,
Ferric chloride, reactions
(dopant; absorption properties of alkoxy-substituted thienylene-vinylene oligomers as a function of the doping level)
- IT 128-08-5, N-Bromosuccinimide 120621-18-3, 3-(Dodecyloxy)thiophene
(monomer synthesis; absorption properties of alkoxy-substituted

- thienylene-vinylene oligomers as a function of the doping level)
- IT 14275-61-7P, (E)-1,2-Bis(tributyltin)ethylene 173291-47-9P,
2,5-Dibromo-3-(dodecyloxy)thiophene 173291-48-0P,
2,5-Dibromo-3,4-bis(dodecyloxy)thiophene 173291-49-1P,
2,5-Dibromo-3,4-dibutoxythiophene 173291-50-4P
(monomer; absorption properties of alkoxy-substituted
thienylene-vinylene oligomers as a function of the doping level)
- IT 173291-51-5P, (E)-1,2-Bis(tributyltin)ethylene-2,5-dibromo-3-
(dodecyloxy)thiophene copolymer 173291-52-6P 173291-53-7P
173291-54-8P 173291-55-9P 174592-80-4P
(oligomeric; absorption properties of alkoxy-substituted
thienylene-vinylene oligomers as a function of the doping level)
- IT 14221-01-3, Tetrakis(triphenylphosphine)palladium(0)
(polymn. catalyst; absorption properties of alkoxy-substituted
thienylene-vinylene oligomers as a function of the doping level)
- IT 77214-82-5P
(polymn. catalyst; absorption properties of alkoxy-substituted
thienylene-vinylene oligomers as a function of the doping level)

L27 ANSWER 24 OF 26 HCA COPYRIGHT 2005 ACS on STN

124:203135 Electrochromic Conducting Polymers via Electrochemical
Polymerization of Bis(2-(3,4-ethylenedioxy)thienyl) Monomers.
Sotzing, Gregory A.; Reynolds, John R.; Steel, Peter J. (Center for
Macromolecular Science and Engineering, University of Florida,
Gainesville, FL, 32611, USA). Chemistry of Materials, 8(4), 882-9
(English) 1996. CODEN: CMATEX. ISSN: 0897-4756. Publisher:
American Chemical Society.

AB A series of bis(2-(3,4-ethylenedioxy)thiophene)-based monomers were
synthesized and fully characterized; specifically
(E)-1,2-bis(2-(3,4-ethylenedioxy)thienyl)vinylene (BEDOT-V),
1,4-bis(2-(3,4-ethylenedioxy)thienyl)benzene (BEDOT-B),
4,4'-bis(2-(3,4-ethylenedioxy)thienyl)biphenyl (BEDOT-BP),
2,5-bis(2-(3,4-ethylenedioxy)thienyl)furan, 2,5-bis(2-(3,4-
ethylenedioxy)thienyl)-thiophene (BEDOT-T), and 2,2':5',2''-ter(3,4-
ethylenedioxy)thiophene, TER-EDOT. The X-ray crystal structures of
BEDOT-V and BEDOT-B were detd. These monomers oxidize and
polymerize at low potentials relative to other reported
electropolymerizable heterocycles. The electroactive polymers
formed have low redox switching potentials and are quite stable in
the conducting state. TER-EDOT had the lowest peak oxidn. potential
of +0.2 V vs Ag/Ag+, making it the most easily oxidized
polymerizable thiophene monomer reported. The electronic band gaps
of these EDOT based polymers were 1.4-2.3 eV (measured as the onset
of the π - π^* transition) offering a diverse range of colors
which may prove useful in electrochromic devices. For example,
poly(BEDOT-V) is deep purple and opaque in the reduced state and
transmissive sky blue in the oxidized state, poly(BEDOT-T) is deep
blue opaque in the reduced state and transmissive blue in the

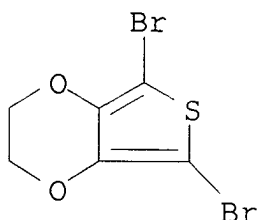
oxidized state, while poly(BEDOT-BP) is transmissive orange in the reduced state and opaque purple in the oxidized state. A thin film of poly(BEDOT-V) switched rapidly between redox states (under 2 s) with an initial optical contrast of 43%. This polymer retained 47% of its optical contrast and 48% of its original charge d. after 600 double potential steps.

IT 174508-31-7P

(intermediate; electrochromic conducting polymers via electrochem. polymn. of bis(ethylenedioxy)thienyl) monomers)

RN 174508-31-7 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro- (9CI) (CA INDEX NAME)



IT Bond angle

Bond length

Crystal structure

Electric conductors, polymeric

(electrochromic conducting polymers via electrochem. polymn. of bis(ethylenedioxy)thienyl) monomers)

IT Polymerization

(electrochem., electrochromic conducting polymers via electrochem. polymn. of bis(ethylenedioxy)thienyl) monomers)

IT Energy level, band structure

(gap, electrochromic conducting polymers via electrochem. polymn. of bis(ethylenedioxy)thienyl) monomers)

IT Polymers, preparation

(polythiophenes, electrochromic conducting polymers via electrochem. polymn. of bis(ethylenedioxy)thienyl) monomers)

IT Crystallography

(x-ray, electrochromic conducting polymers via electrochem. polymn. of bis(ethylenedioxy)thienyl) monomers)

IT 162899-00-5P 168641-47-2P 168641-48-3P 174508-35-1P

174508-36-2P 174508-37-3P

(electrochromic conducting polymers via electrochem. polymn. of bis(ethylenedioxy)thienyl) monomers)

IT 32460-00-7P, 2,5-Dibromofuran. 162898-99-9P 168641-43-8P

174508-31-7P

(intermediate; electrochromic conducting polymers via electrochem. polymn. of bis(ethylenedioxy)thienyl) monomers)

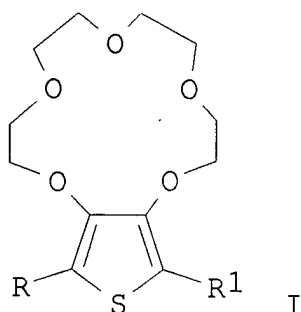
IT 168641-44-9P 174508-32-8P 174508-33-9P 174508-34-0P
(monomer; electrochromic conducting polymers via electrochem.
polymn. of bis(ethylenedioxy)thienyl) monomers)

IT 106-37-6, p-Dibromobenzene. 110-00-9, Furan 156-60-5
3141-27-3, 2,5-Dibromothiophene 126213-50-1, 3,4-
Ethylenedioxythiophene
(starting material; electrochromic conducting polymers via
electrochem. polymn. of bis(ethylenedioxy)thienyl) monomers)

L27 ANSWER 25 OF 26 HCA COPYRIGHT 2005 ACS on STN

122:315261 Synthesis and characterization of thiophenes, oligothiophenes
and polythiophenes with crown ether units in direct
 π -conjugation. Baeuerle, P.; Scheib, St. (Inst. Organische
Chemie, Universitaet Wuerzburg, Wuerzburg, D-97074, Germany). Acta
Polymerica, 46(2), 124-9 (English) 1995. CODEN: ACPODY. ISSN:
0323-7648. Publisher: VCH.

GI



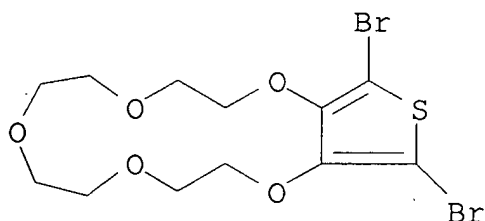
AB I ($R, R' = 2$ -thiophenyl; $R, R' = H$; $R = H, R' = 2$ -thiophenyl) were
prepd. by substitution of I ($R, R' = Br$) with 2-
(trimethylstannyl)thiophene, deacylation of I ($R, R' =$
ethyloxycarbonyl), and substitution of I ($R = H, R' =$
trimethylstannyl). I ($R, R' = H$; $R = H, R' = 2$ -thiophenyl) were
polymd. potentiodynamically to prep. selectively conducting
polythiophenes with crown ether units in direct π -conjugation.
The redox behavior of polymer films was characterized by cyclic
voltammograms in MeCN solns. in the presence of Li^+ , Na^+ , and K^+
cations, and by spectroelectrochem. measurements. The redox
behavior of I ($R, R' = H$) polymer was effected by the introduction of
cations, whereas that of I ($R = H, R' = 2$ -thiophenyl) polymer was
not. The sensitivity of I ($R, R' = H$) polymer to cations increased
in the order: $Na^+ \gg Li^+ > K^+$.

IT 163657-74-7P

(prepn. and electrochem. properties of thiophenes and polythiophenes with crown ether units in direct π -conjugation)

RN 163657-74-7 HCA

CN Thieno[3,4-b]-1,4,7,10,13-pentaoxacyclopentadecin,
14,16-dibromo-2,3,5,6,8,9,11,12-octahydro- (9CI) (CA INDEX NAME)



IT Electric conductors, polymeric
Electric current

(prepn. and electrochem. properties of thiophenes and polythiophenes with crown ether units in direct π -conjugation)

IT Polymerization

(electrochem., prepn. and electrochem. properties of thiophenes and polythiophenes with crown ether units in direct π -conjugation)

IT Electric potential

(oxidn., prepn. and electrochem. properties of thiophenes and polythiophenes with crown ether units in direct π -conjugation)

IT Polymers, preparation

(polythiophenes, crown ether group-contg., prepn. and electrochem. properties of thiophenes and polythiophenes with crown ether units in direct π -conjugation)

IT 3109-63-5, Tetrabutylammonium hexafluorophosphate 7601-89-0,
Sodium perchlorate 7791-03-9, Lithium perchlorate 17084-13-8,
Potassium hexafluorophosphate

(prepn. and electrochem. properties of thiophenes and polythiophenes with crown ether units in direct π -conjugation)

IT 163657-76-9P 163657-77-0P

(prepn. and electrochem. properties of thiophenes and polythiophenes with crown ether units in direct π -conjugation)

IT 163657-78-1P 163657-79-2P

(prepn. and electrochem. properties of thiophenes and polythiophenes with crown ether units in direct π -conjugation)

IT 1066-45-1, Trimethylstannyl chloride 3437-95-4, 2-Iodothiophene
37496-13-2, 2-(Trimethylstannyl)thiophene 122372-64-9

(prepn. and electrochem. properties of thiophenes and polythiophenes with crown ether units in direct π -conjugation)

IT 163657-75-8P

(prepn. and electrochem. properties of thiophenes and polythiophenes with crown ether units in direct π -conjugation)

IT 163657-74-7P

(prepn. and electrochem. properties of thiophenes and polythiophenes with crown ether units in direct π -conjugation)

L27 ANSWER 26 OF 26 HCA COPYRIGHT 2005 ACS on STN

69:35839 Synthesis in the thiophene series. Morel, Jean; Pastour, Paul (Lab. Chim. Org., Fac. Sci. Rouen, Mont-St.-Aignan, Fr.). Bulletin de la Societe Chimique de France (2), 737-8 (French) 1968. CODEN: BSCFAS. ISSN: 0037-8968.

GI For diagram(s), see printed CA Issue.

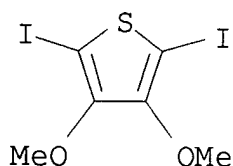
AB Treatment of I (R = CO₂H) with SOCl₂ gave I (R = COCl), m. 94°, which was treated with NH₃ in ether soln. to give 74% I (R = CONH₂) (II), m. 247°. II was treated with POCl₃ to give 90% I (R = CN), m. 132°, which was reduced with LiAlH₄ to give 43% I (R = CHO), m. 122°. A mixt. of 2.8 g. I (R = CO₂H) and 16 g. Hg(OAc)₂ in 50 cc. HOAc was refluxed 15 min., mixed with a slight excess of iodine, and extd. with ether to give 19% I (R = I) (III), m. 74°. III treated with BuLi followed by HCONMe₂ gave 37% I (R = CHO), and with MeCONMe₂ gave 35% I (R = Ac), m. 182°.

IT 19848-31-8P

(prepn. of)

RN 19848-31-8 HCA

CN Thiophene, 2,5-diiodo-3,4-dimethoxy- (8CI) (CA INDEX NAME)



IT 19848-26-1P 19848-27-2P 19848-28-3P 19848-29-4P 19848-30-7P

19848-31-8P 19889-07-2P

(prepn. of)

=> d 128 1-4 ti

L28 ANSWER 1 OF 4 HCA COPYRIGHT 2005 ACS on STN

TI Characterization of Organic p/n Junction Photodiodes Based on Poly(alkylthiophene)/Perylene Diimide Bilayers

L28 ANSWER 2 OF 4 HCA COPYRIGHT 2005 ACS on STN

TI Optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers

L28 ANSWER 3 OF 4 HCA COPYRIGHT 2005 ACS on STN

TI Temperature-dependent electrical conductivity of p-doped poly(3,4-ethylenedioxythiophene) and poly(3-alkylthiophene)s

L28 ANSWER 4 OF 4 HCA COPYRIGHT 2005 ACS on STN

TI Methylenedioxyhetarenes. 2. Reactions of diethyl 3,4-methylenedioxy-2,5-thiophenedicarboxylate

=> d 128 1-4 cbib abs hitstr it

L28 ANSWER 1 OF 4 HCA COPYRIGHT 2005 ACS on STN

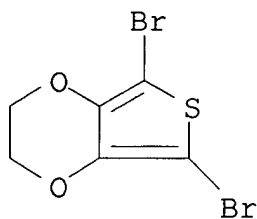
139:93393 Characterization of Organic p/n Junction Photodiodes Based on Poly(alkylthiophene)/Perylene Diimide Bilayers. Tan, Li; Curtis, M. David; Francis, A. H. (Macromolecular Science & Engineering Center and Department of Chemistry, The University of Michigan, Ann Arbor, MI, 48109-1055, USA). Chemistry of Materials, 15(11), 2272-2279 (English) 2003. CODEN: CMATEX. ISSN: 0897-4756. Publisher: American Chemical Society.

AB Photoconduction of bilayer org. p/n junction photocells can be finely tuned through the alteration of either the side chain orientation (regiorandom vs. regioregular) or main chain structure in poly(3-alkylthiophene)s (P3ATs), where the incorporation of an electron-donating group (EDOT) appears to be an excellent method for enhancing the photoconduction. also, doping of P3ATs proved to be an equally viable route for tuning the device characteristics. These polymers were used to fabricate bilayer org. photocells with the polymer as the p-type layer and 1,2-diaminobenzeneperylene-3,4,9,10-tetracarboxylic acid diimide (PV) as the n-type layer. Action spectra at steady-state illumination demonstrated that all the interfaces (org.-org. p/n junction and org.-electrode) are actively involved in the photogeneration of carriers. Crit. device properties, for example, open-circuit voltage (Voc) and short-circuit current (Isc), are not only dependent on the selection of electrodes and org. materials but also greatly affected by the illumination wavelength and intensity.

IT 174508-31-7P, 2,5-Dibromo-3,4-ethylenedioxythiophene (prepn. of)

RN 174508-31-7 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro- (9CI) (CA INDEX NAME)



- IT Electric current carriers
(generation; properties of org. pn photodiodes based on polyalkylthiophenes and diaminobenzeneperylenetetracarboxylic acid diimide)
- IT Glass substrates
(in fabrication of org. pn photodiodes based on polyalkylthiophenes and diaminobenzeneperylenetetracarboxylic acid diimide)
- IT Cyclic voltammetry
(of polyalkylthiophene derivs.)
- IT Band gap
(optical; of polyalkylthiophene derivs.)
- IT Conducting polymers
(polythiophenes; properties of org. pn photodiodes based on polyalkylthiophenes and diaminobenzeneperylenetetracarboxylic acid diimide)
- IT Absorption spectra
- Dopants
- Electric current-potential relationship
- Electrodes
- Open circuit potential
- Optical absorption
- Photoconductivity
- Photocurrent
- Photodiodes
- Short circuits
- Solid-solid interface
(properties of org. pn photodiodes based on polyalkylthiophenes and diaminobenzeneperylenetetracarboxylic acid diimide)
- IT Coating process
(spin; in fabrication of org. pn photodiodes based on polyalkylthiophenes and diaminobenzeneperylenetetracarboxylic acid diimide)
- IT 104-15-4, Toluenesulfonic acid, uses 7647-01-0, Hydrogen chloride, uses 7664-93-9, Sulfuric acid, uses 14635-75-7, Nitrosonium tetrafluoroborate
(P3OT dopant; properties of org. pn photodiodes based on polyalkylthiophenes and diaminobenzeneperylenetetracarboxylic acid diimide)

- acid diimide)
- IT 98837-51-5, Poly(3-butylthiophene)
(UV spectra of)
- IT 7440-22-4, Silver, uses
(contact; properties of org. pn photodiodes based on
polyalkylthiophenes and diaminobenzeneperylenetetracarboxylic
acid diimide)
- IT 116971-10-9, 2,5-Dibromo-3-butylthiophene
(in prepn. of butylthiophene-ethylenedioxythiophene copolymer)
- IT 126213-50-1, 3,4-Ethylenedioxythiophene
(in prepn. of dibromoethylenedioxythiophene)
- IT 554459-31-3P, 2,5-Dibromo-3-butylthiophene-2,5-dibromo-3,4-
ethylenedioxythiophene copolymer
(prepn. and properties of)
- IT 174508-31-7P, 2,5-Dibromo-3,4-ethylenedioxythiophene
(prepn. of)
- IT 50926-11-9, ITO 55034-79-2
(properties of org. pn photodiodes based on polyalkylthiophenes
and diaminobenzeneperylenetetracarboxylic acid diimide)
- IT 104934-51-2, Poly(3-octylthiophene)
(pure and doped; properties of org. pn photodiodes based on
polyalkylthiophenes and diaminobenzeneperylenetetracarboxylic
acid diimide)
- IT 7664-41-7, Ammonia, processes
(redn. of doped P3OT with; properties of org. pn photodiodes
based on polyalkylthiophenes and diaminobenzeneperylenetetracarbo
xylic acid diimide)

L28 ANSWER 2 OF 4 HCA COPYRIGHT 2005 ACS on STN

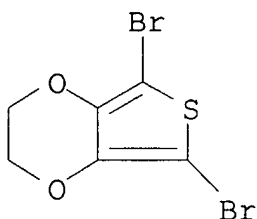
137:232315 Optical and redox properties of a series of
3,4-ethylenedioxythiophene oligomers. Apperloo, Joke J.;
Groenendaal, L. "Bert"; Verheyen, Hilde; Jayakannan, Manickam;
Janssen, Rene A. J.; Dkhissi, Ahmed; Beljonne, David; Lazzaroni,
Roberto; Bredas, Jean-Luc (Laboratory for Macromolecular and Organic
Chemistry, Eindhoven University of Technology, Eindhoven, 5600 MB,
Neth.). Chemistry--A European Journal, 8(10), 2384-2396 (English)
2002. CODEN: CEUJED. ISSN: 0947-6539. OTHER SOURCES: CASREACT
137:232315. Publisher: Wiley-VCH Verlag GmbH.

AB The optical and redox properties of a series of 3,4-
ethylenedioxythiophene oligomers (EDOT_n, n = 1-4) and their
β,β'-unsubstituted analogs (T_n, n = 1-4) are described.
Both series are end capped with Ph groups to prevent irreversible
α-coupling reactions during oxidative doping. Absorption and
fluorescence spectra of both series reveal a significantly higher
degree of intrachain conformational order in the EDOT_n oligomers.
Oxidn. potentials (EPA1 and EPA2) detd. by cyclic voltammetry reveal
that those of EDOT_n are significantly lower than the corresponding
T_n oligomers as a consequence of the electron-donating

3,4-ethylenedioxy substitution. Linear fits of EPA1 and EPA2 vs. the reciprocal no. of double bonds reveal significantly steeper slopes for the EDOTn than for the Tn oligomers. This could indicate a more effective conjugation for the EDOTn series, confirmed by the fact that coalescence of EPA1 and EPA2 is reached already at relatively short chain lengths (≈ 5 EDOT units) in contrast to the Tn series (> 10 thiophene units). The stepwise chem. oxidn. of the EDOTn and Tn oligomers in soln. was carried out to obtain radical cations and dications. The energies of the optical transitions of the radical cations and dications as detd. by UV/Vis/NIR spectroscopy were similar for the two series. These spectroscopic observations are consistent with quantum-chem. calcns. performed on the singly charged mols. Cooling solns. contg.

T2 $\bullet+$, T3 $\bullet+$, EDOT2 $\bullet+$, and EDOT3 $\bullet+$ revealed the reversible formation of dimers, albeit with a some-what different tendency, expressed in the values for the dimerization enthalpy.

IT 174508-31-7P, 2,5-Dibromo-3,4-ethylenedioxythiophene
(coupling; prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
RN 174508-31-7 HCA
CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro- (9CI) (CA INDEX NAME)



IT Radical ions
(cations, formation, electronic and ESR spectra, and dimerization; prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
IT Exciton
(coupling in radical cation dimers; prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
IT Cations
(divalent; prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
IT Substituent effects
(ethylenedioxy; prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
IT CI (molecular orbital method)
Oscillator strength
(in electronic excitation of radical cations; prepn. and optical

- and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
- IT Conformation
(intrachain conformational order; prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
- IT Dimerization
Dimerization enthalpy
ESR (electron spin resonance)
Electronic excitation
Hyperfine coupling
(of radical cations; prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
- IT Chemical chains
Fluorescence
Homologous series
Oxidation potential
UV and visible spectra
Vibronic excitation
(prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
- IT Oligomers
(prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
- IT Conjugation (bond)
(π -; prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
- IT 29488-24-2, 2-Bromo-5-phenylthiophene
(boronation; prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
- IT 591-50-4, Iodobenzene 625-88-7, 2,5-Diiodothiophene 3339-80-8,
5,5'-Diiodo-2,2'-bithiophene 24388-23-6 104499-99-2,
5,5''-Diiodo-2,2':5',2''-terthiophene 264282-36-2
(coupling; prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
- IT **174508-31-7P**, 2,5-Dibromo-3,4-ethylenedioxythiophene
459409-70-2P 459409-71-3P 459409-73-5P 459409-74-6P
(coupling; prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
- IT 76-09-5, Pinacol
(cyclocondensation with boronic acid; prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
- IT 205436-42-6 459409-82-6
(dimerization; prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
- IT 1665-32-3P, 5,5''-Diphenyl-2,2':5',2''-terthiophene 83495-30-1P,
5,5'-Diphenyl-2,2'-bithiophene 459409-75-7P 459409-76-8P
459409-77-9P

- (electro- and chem. oxidn.; prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
- IT 238397-97-2P, 5,5'''-Diphenyl-2,2':5',2'':5'',2'''-quaterthiophene (electro- and chem. oxidn.; prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
- IT 1445-78-9P, 2,5-Diphenylthiophene 459409-78-0P (electrooxidn.; prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
- IT 185258-96-2 459409-83-7 (oxidn. and dimerization; prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
- IT 459409-85-9 (oxidn.; prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
- IT 459409-79-1P 459409-80-4P (prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
- IT 459409-81-5 459409-84-8 459409-86-0 459409-87-1 459409-88-2 (prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
- IT 98-80-6, Phenylboronic acid (prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
- IT 126213-50-1, 3,4-Ethylenedioxythiophene (reactions; prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
- IT 459409-72-4P (reactions; prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)
- IT 195602-17-6 (stannylation; prepn. and optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers)

L28 ANSWER 3 OF 4 HCA COPYRIGHT 2005 ACS on STN

131:5811 Temperature-dependent electrical conductivity of p-doped poly(3,4-ethylenedioxythiophene) and poly(3-alkylthiophene)s. Yamamoto, Takakazu; Abia, Mahmut; Shimizu, Takahisa; Komarudin, Dahrma; Lee, Bang-Lin; Kurokawa, Eriko (Research Laboratory Resources Utilization, Tokyo Institute Technology, Yokohama, 226, Japan). Polymer Bulletin (Berlin), 42(3), 321-327 (English) 1999. CODEN: POBUDR. ISSN: 0170-0839. Publisher: Springer-Verlag.

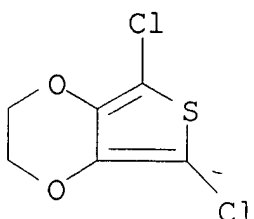
AB Temp.-dependent elec. cond. of the substituted polythiophenes poly(3,4-ethylenedioxythiophene) (PEDOT_h) and head-to-tail type poly(3-alkylthiophene) (HT-P3RTh) was measured. The elec. cond. (σ) of p-doped PEDOT_h and HT-P3RTh obeys equations of a type, $\ln \sigma = \ln \sigma_0 - (T_0/T)0.25$, with the T_0 value of ≈ 105 - 107 K.

IT 225518-49-0P

(monomer; temp.-dependent elec. cond. of p-doped substituted polythiophenes)

RN 225518-49-0 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dichloro-2,3-dihydro- (9CI) (CA INDEX NAME)



- IT Polymers, properties
(polythiophenes; temp.-dependent elec. cond. of p-doped substituted polythiophenes)
- IT Conducting polymers
Electric conductivity
(temp.-dependent elec. cond. of p-doped substituted polythiophenes)
- IT 7553-56-2, Iodine, uses 14946-92-0, Iron tetrachloride
(dopant; temp.-dependent elec. cond. of p-doped substituted polythiophenes)
- IT 110134-47-9, Poly(3-hexyl-2,5-thiophenediyl) 135899-67-1,
3-Thiophenepropanesulfonic acid homopolymer 216318-88-6,
Poly(3-methyl-2,5-thiophenediyl)
(doped; temp.-dependent elec. cond. of p-doped substituted polythiophenes)
- IT 126213-50-1P
(in prepn. of dichloro thiophene monomer)
- IT 163359-60-2P 225518-50-3P
(iodine- and iron tetrachloride-doped; temp.-dependent elec. cond. of p-doped substituted polythiophenes)
- IT **225518-49-0P**
(monomer; temp.-dependent elec. cond. of p-doped substituted polythiophenes)

L28 ANSWER 4 OF 4 HCA COPYRIGHT 2005 ACS on STN

82:170765 Methyleneedioxyhetarenes. 2. Reactions of diethyl 3,4-methyleneedioxy-2,5-thiophenedicarboxylate. Dallacker, Franz; Mues, Volker (Inst. Org. Chem., Tech. Hochsch. Aachen, Aachen, Fed. Rep. Ger.). Chemische Berichte, 108(2), 576-81 (German) 1975. CODEN: CHBEAM. ISSN: 0009-2940. OTHER SOURCES: CASREACT 82:170765.

GI For diagram(s), see printed CA Issue.

AB The sym. thiophene deriv. I (R = R1 = CO2Et) (II) was treated with excess alc. KOH, N2H4.H2O, and Br at pH 7.0 to give .apprx.100% I (R

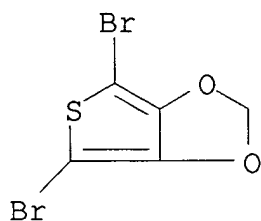
= R1 = CO2H) (III), 79% I (R = R1 = CONHNH2) (IV), and extremely light- and air-sensitive I (R = R1 = Br) (V), resp. III was esterified to give I (R = R1 = CO2Me) or chlorinated and aminated, e.g. with NH3, to give I (R = R1 = CONH2) (VI). IV was condensed with piperonal to yield the piperonylidene deriv. I (R = R1 = CONHN:CHC6H3O2CH2-3,4) and V converted into I (R = R1 = iodo). Boiling VI and POCl3 gave 54% I (R = R1 = CN), which with H2S in pyridine-Et3N gave 100% I (R = R1 = CSNH2).

IT 55370-18-8P 55370-19-9P

(prepn. of)

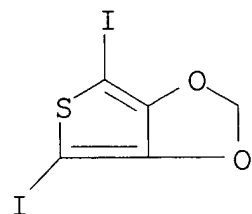
RN 55370-18-8 HCA

CN Thieno[3,4-d]-1,3-dioxole, 4,6-dibromo- (9CI) (CA INDEX NAME)



RN 55370-19-9 HCA

CN Thieno[3,4-d]-1,3-dioxole, 4,6-diiodo- (9CI) (CA INDEX NAME)



IT 55370-05-3

(bromination and hydrazinolysis and hydrolysis of)

IT 55370-20-2P

(prepn. and decarboxylation and esterification and reaction with thionyl chloride)

IT 55370-12-2P 55370-24-6P

(prepn. and dehydration of)

IT 55370-26-8P 55370-28-0P

(prepn. and hydrolysis of)

IT 55370-11-1P

(prepn. and reaction with amines)

IT 55370-06-4P

(prepn. and reaction with bromine and methanol and thionyl chloride)

IT 55370-08-6P

(prepn. and reaction with piperonal)
IT 55370-30-4P
(prepn. and reaction with sodium sulfide)
IT 55370-07-5P 55370-09-7P 55370-10-0P 55370-13-3P 55370-14-4P
55370-15-5P 55370-16-6P 55370-17-7P **55370-18-8P**
55370-19-9P 55370-21-3P 55370-22-4P 55370-23-5P
55370-25-7P 55370-27-9P 55370-29-1P 55370-31-5P
(prepn. of)
IT 120-57-0
(reaction of, with (methylenedioxy)thiophenecarbohydrazide)
IT 100-61-8
(reaction of, with (methylenedioxy)thiophenedicarboxylic acid)
IT 30525-89-4
(reaction of, with dibromobutanediol)
IT 14396-65-7
(reaction of, with formaldehyde)
IT 110-89-4, reactions
(with (methylenedioxy)thiophenedicarboxylic acid)

=> d 126 1-29 cbib abs hitstr it

L26 ANSWER 1 OF 29 HCA COPYRIGHT 2005 ACS on STN

141:380500 Spray Coatable Electrochromic Dioxothiophene Polymers with High Coloration Efficiencies. Reeves, Benjamin D.; Grenier, Christophe R. G.; Argun, Avni A.; Cirpan, Ali; McCarley, Tracy D.; Reynolds, John R. (Department of Chemistry, Center for Macromolecular Science and Engineering, University of Florida, Gainesville, FL, 32611-7200, USA). *Macromolecules*, 37(20), 7559-7569 (English) 2004. CODEN: MAMOBX. ISSN: 0024-9297. Publisher: American Chemical Society.

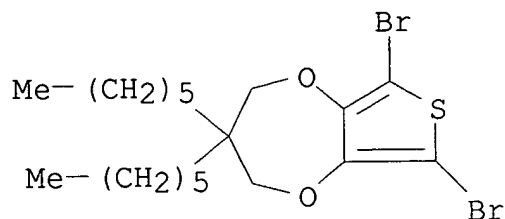
AB Four new disubstituted propylenedioxothiophene polymers have been synthesized by Grignard metathesis on the 1-5 g scale. All polymers were found to be sol. in chloroform, methylene chloride, toluene, and THF and were fully structurally characterized having GPC detd. no.-av. mol. wts. ranging from 33000 to 47000 g mol⁻¹. Dil. polymer solns. in toluene exhibited strong red fluorescence with moderate quantum efficiencies from 0.38 to 0.50. Homogeneous thin films were formed by electropolymerization and spray casting polymer solns. onto ITO coated glass slides at thicknesses of ca. 150 nm. The films were electroactive, switching from a dark blue-purple to a transmissive sky blue upon p-doping, often with subsecond switching times, and high electrochromic contrast luminance changes (% ΔY) of 40-70%. These studies revealed that the branched derivs., [poly(3,3-bis(2-ethylhexyl)-3,4-dihydro-2H-thieno[3,4-b][1,4]dioxepine)] and [poly(6,8-dibromo-3,3-bis(2-ethylhexyloxymethyl)-3,4-dihydro-2H-thieno[3,4-b][1,4]dioxepine)], gave an electrochem. response and assocd. color change over a much smaller voltage range in comparison to the linear chain substituted derivs., [poly(3,3-dihexyl-3,4-dihydro-2H-thieno[3,4-b][1,4]dioxepine)] and [poly(3,3-bis(octadecyloxymethyl)-3,4-dihydro-2H-thieno[3,4-b][1,4]dioxepine)]. Composite coloration efficiency values were found up to 1365 cm²/C; this was considerably larger than values obtained from previously studied alkylenedioxothiophene based polymers (.apprx.375 cm²/C).

IT 700817-04-5P 700817-06-7P 700817-08-9P
700817-10-3P

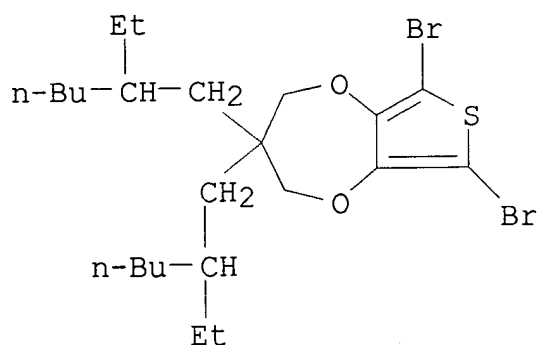
(monomer; prepn. and electrooptical properties of spray coatable electrochromic dioxothiophene polymers)

RN 700817-04-5 HCA

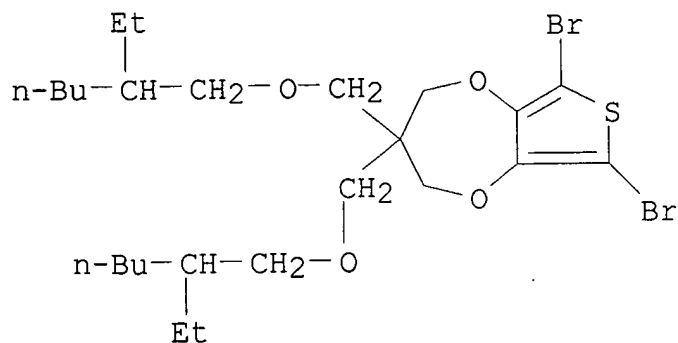
CN 2H-Thieno[3,4-b][1,4]dioxepin, 6,8-dibromo-3,3-dihexyl-3,4-dihydro-
(9CI) (CA INDEX NAME)



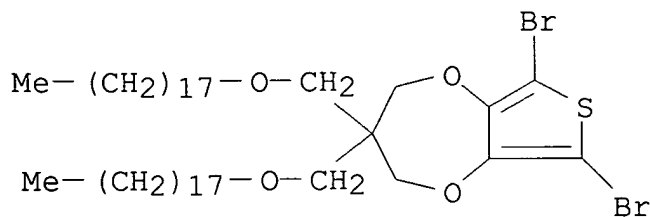
RN 700817-06-7 HCA
 CN 2H-Thieno[3,4-b][1,4]dioxepin, 6,8-dibromo-3,3-bis(2-ethylhexyl)-3,4-dihydro- (9CI) (CA INDEX NAME)



RN 700817-08-9 HCA
 CN 2H-Thieno[3,4-b][1,4]dioxepin, 6,8-dibromo-3,3-bis[[(2-ethylhexyl)oxy]methyl]-3,4-dihydro- (9CI) (CA INDEX NAME)



RN 700817-10-3 HCA
 CN 2H-Thieno[3,4-b][1,4]dioxepin, 6,8-dibromo-3,4-dihydro-3,3-bis[(octadecyloxy)methyl]- (9CI) (CA INDEX NAME)



IT 700817-12-5P 700817-14-7P 700817-16-9P
 700817-18-1P 783322-80-5P 783322-81-6P
 783322-82-7P 783322-83-8P

(prepn. and electrooptical properties of spray coatable
 electrochromic dioxothiophene polymers)

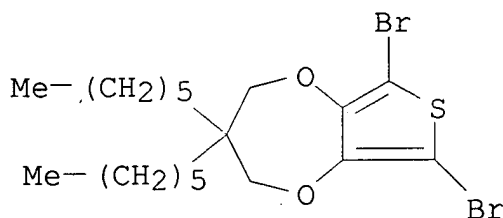
RN 700817-12-5 HCA

CN 2H-Thieno[3,4-b][1,4]dioxepin, 6,8-dibromo-3,3-diethyl-3,4-dihydro-,
 homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 700817-04-5

CMF C19 H30 Br2 O2 S



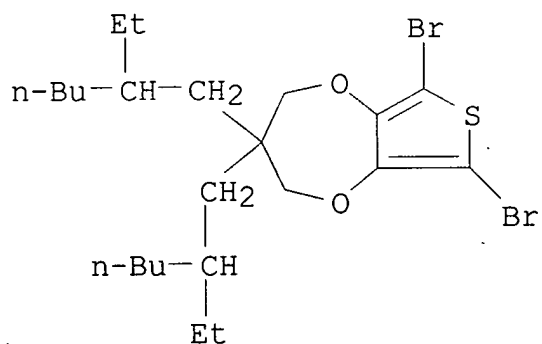
RN 700817-14-7 HCA

CN 2H-Thieno[3,4-b][1,4]dioxepin, 6,8-dibromo-3,3-bis(2-ethylhexyl)-3,4-
 dihydro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 700817-06-7

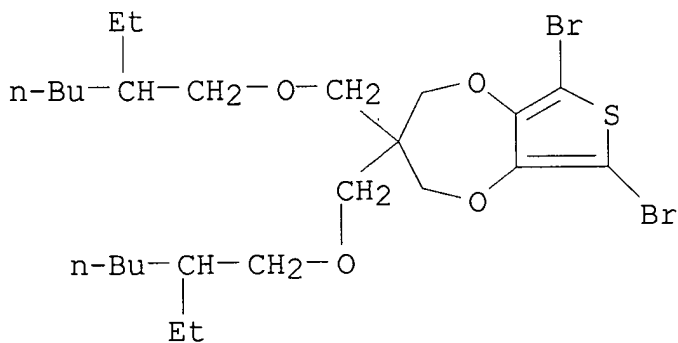
CMF C23 H38 Br2 O2 S



RN 700817-16-9 HCA
 CN 2H-Thieno[3,4-b][1,4]dioxepin, 6,8-dibromo-3,3-bis[[(2-ethylhexyl)oxy]methyl]-3,4-dihydro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

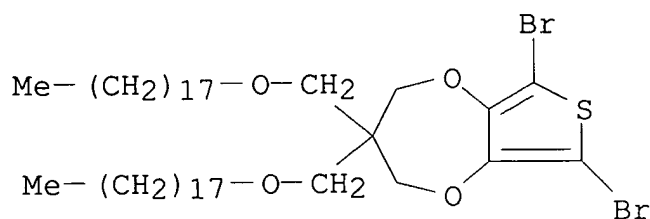
CRN 700817-08-9
 CMF C25 H42 Br2 O4 S



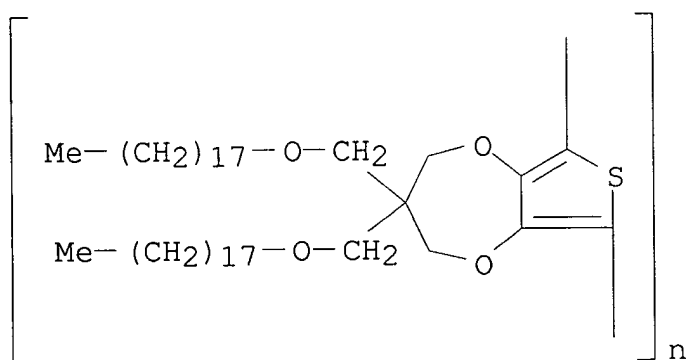
RN 700817-18-1 HCA
 CN 2H-Thieno[3,4-b][1,4]dioxepin, 6,8-dibromo-3,4-dihydro-3,3-bis[(octadecyloxy)methyl]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

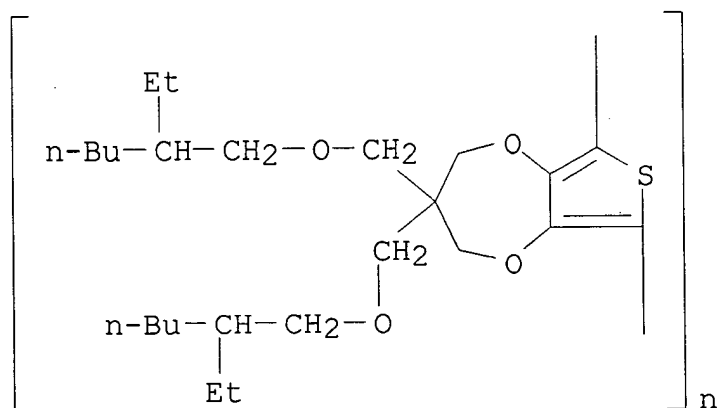
CRN 700817-10-3
 CMF C45 H82 Br2 O4 S



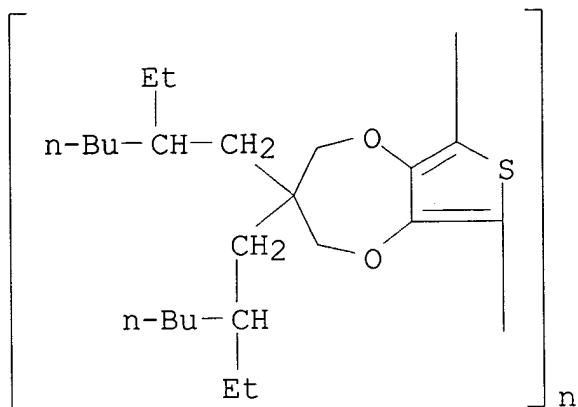
RN 783322-80-5 HCA
 CN Poly[3,4-dihydro-3,3-bis[(octadecyloxy)methyl]-2H-thieno[3,4-b][1,4]dioxepin-6,8-diyl] (9CI) (CA INDEX NAME)



RN 783322-81-6 HCA
 CN Poly[3,3-bis[[2-ethylhexyl)oxy]methyl]-3,4-dihydro-2H-thieno[3,4-b][1,4]dioxepin-6,8-diyl] (9CI) (CA INDEX NAME)

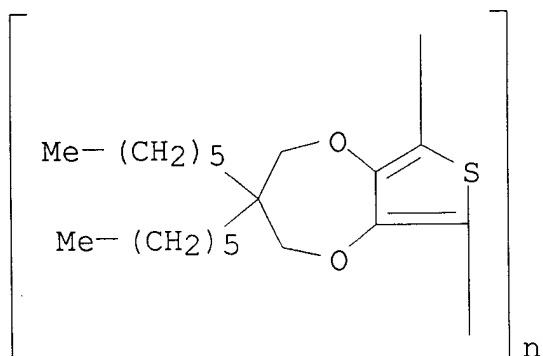


RN 783322-82-7 HCA
 CN Poly[3,3-bis(2-ethylhexyl)-3,4-dihydro-2H-thieno[3,4-b][1,4]dioxepin-6,8-diyl] (9CI) (CA INDEX NAME)



RN 783322-83-8 HCA

CN Poly(3,3-dihexyl-3,4-dihydro-2H-thieno[3,4-b][1,4]dioxepin-6,8-diyl)
(9CI) (CA INDEX NAME)



- IT Polymerization
(Grignard; prepn. and electrooptical properties of spray coatable electrochromic dioxothiophene polymers)
- IT Polymerization
(electrochem.; prepn. and electrooptical properties of spray coatable electrochromic dioxothiophene polymers)
- IT Band gap
(optical; prepn. and electrooptical properties of spray coatable electrochromic dioxothiophene polymers)
- IT Conducting polymers
(polythiophenes; prepn. and electrooptical properties of spray coatable electrochromic dioxothiophene polymers)
- IT Electrochromism
Luminescence, electroluminescence
Redox potential
(prepn. and electrooptical properties of spray coatable

- electrochromic dioxythiophene polymers)
- IT Electrooptical effect
(switching; prepn. and electrooptical properties of spray
coatable electrochromic dioxythiophene polymers)
- IT 104-76-7, 2-Ethyl-1-hexanol 105-53-3, Diethyl malonate 111-25-1,
Hexyl bromide 112-92-5, 1-Octadecanol 3296-90-0,
2,2-Di(bromomethyl)-1,3-diol 18908-66-2, 2-Ethylhexyl bromide
51792-34-8, 3,4-Dimethoxythiophene
(monomer synthesis; prepn. and electrooptical properties of spray
coatable electrochromic dioxythiophene polymers)
- IT 54662-33-8P 634591-75-6P 634591-77-8P 700816-90-6P
701209-98-5P
(monomer synthesis; prepn. and electrooptical properties of spray
coatable electrochromic dioxythiophene polymers)
- IT 700816-98-4P 700817-00-1P 700817-04-5P
700817-06-7P 700817-08-9P 700817-10-3P
(monomer; prepn. and electrooptical properties of spray coatable
electrochromic dioxythiophene polymers)
- IT 700817-12-5P 700817-14-7P 700817-16-9P
700817-18-1P 783322-80-5P 783322-81-6P
783322-82-7P 783322-83-8P
(prepn. and electrooptical properties of spray coatable
electrochromic dioxythiophene polymers)

L26 ANSWER 2 OF 29 HCA COPYRIGHT 2005 ACS on STN

141:314660 Synthesis and polymerization of perfluoroalkylated
3,4-propylenedioxythiophene. Dong, Jian-Hai; Meng, Wei-Dong; Qing,
Feng-Ling (Coll. Chem. Chem. Eng., Donghua Univ., Shanghai, 200051,
Peop. Rep. China). ARKIVOC (Gainesville, FL, United States) (9),
9-14 (English) 2004. CODEN: AGFUAR. URL: <http://www.arkat-usa.org/ark/journal/2004/Yuan/CY-1037L/CY-1037L.pdf> Publisher:
Arkats USA Inc..

AB A novel monomer, perfluoroalkylated 3,4-propylenedioxythiophene, was
prepd. by trans-etherification reaction between 3,4-
dimethoxythiophene and perfluoroalkylated cycloalkylpropane-1,3-
diol. Bromination of monomer followed by a Grignard metathesis
coupling reaction provided perfluoroalkylated poly(3,4-
propylenedioxythiophene). This polymer was quite insol. in any
known solvent.

IT 768400-96-0P
(multi-step prepn. of perfluoroalkylated propylenedioxythiophene
monomer and its bromination followed by Grignard metathesis
coupling polymn.)

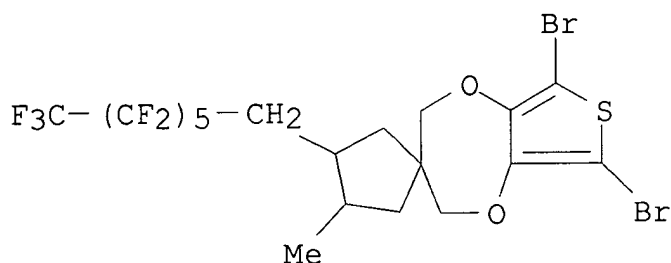
RN 768400-96-0 HCA

CN Spiro[cyclopentane-1,3'-(4'H)-[2H]thieno[3,4-b][1,4]dioxepin],
6',8'-dibromo-3-methyl-4-(2,2,3,3,4,4,5,5,6,6,7,7,7-
tridecafluoroheptyl)-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 768400-95-9

CMF C19 H15 Br2 F13 O2 S



- IT Polymerization
(Grignard, metathetic; multi-step prepn. of perfluoroalkylated propylenedioxythiophene monomer and its bromination followed by Grignard metathesis coupling polymn.)
- IT Polymerization
(metathetic, Grignard; multi-step prepn. of perfluoroalkylated propylenedioxythiophene monomer and its bromination followed by Grignard metathesis coupling polymn.)
- IT 3195-24-2P, Diethyl 2,2-diallylmalonate
(cyclization of; multi-step prepn. of perfluoroalkylated propylenedioxythiophene monomer and its bromination followed by Grignard metathesis coupling polymn.)
- IT 768400-93-7P
(cycloaddn. of; multi-step prepn. of perfluoroalkylated propylenedioxythiophene monomer and its bromination followed by Grignard metathesis coupling polymn.)
- IT 105-53-3, Diethyl malonate 106-95-6, Allyl bromide, reactions
355-43-1, Perfluorohexyl iodide 51792-34-8, 3,4-Dimethoxythiophene
(multi-step prepn. of perfluoroalkylated propylenedioxythiophene monomer and its bromination followed by Grignard metathesis coupling polymn.)
- IT 768400-94-8P 768400-95-9P
(multi-step prepn. of perfluoroalkylated propylenedioxythiophene monomer and its bromination followed by Grignard metathesis coupling polymn.)
- IT **768400-96-0P**
(multi-step prepn. of perfluoroalkylated propylenedioxythiophene monomer and its bromination followed by Grignard metathesis coupling polymn.)
- IT 169893-13-4P
(redn. of; multi-step prepn. of perfluoroalkylated propylenedioxythiophene monomer and its bromination followed by Grignard metathesis coupling polymn.)

L26 ANSWER 3 OF 29 HCA COPYRIGHT 2005 ACS on STN

141:89456 Copolymers of 3,4-Ethylenedioxythiophene and of Pyridine Alternated with Fluorene or Phenylene Units: Synthesis, Optical Properties, and Devices. Aubert, Pierre-Henri; Knipper, Martin; Groenendaal, Lambertus; Lutsen, Laurence; Manca, Jean; Vanderzande, Dirk (IMOMEC Division, IMEC, Diepenbeek, B-3590, Belg.). Macromolecules, 37(11), 4087-4098 (English) 2004. CODEN: MAMOBX. ISSN: 0024-9297. Publisher: American Chemical Society.

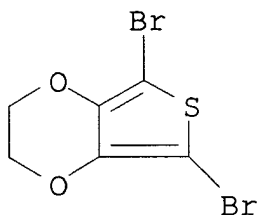
AB We report the synthesis of four conjugated copolymers based on alkylated fluorene or phenylene units which band gap is tuned by the regular insertion of an electron-donating or electron-withdrawing unit, (3,4-ethylenedioxy)thiophene and pyridine, resp. The (AB)_n regular sequence is achieved by Suzuki polycondensation reactions. The characterization of the copolymers by size exclusion chromatog. reveals chains lengths of about 20-30 repeat units (40-60 rings), leading to a good processability for potential optical applications. The 1:1 ratio between the two units improves the soly. of the material in common org. solvents, allowing for physicochem. characterizations. Raman and FT-IR expts. indicate that the electronic structure of the backbone is rather benzenic in the neutral (undoped) state, as opposed to a quinoic oxidized structure. All copolymers exhibit interesting electrochromic properties as attested by cyclic voltammetry and UV-vis expts. They reversibly switch among the entire visible spectra, which is of particular importance for display applications. Moreover, the EDOT-based copolymers strongly absorb in the NIR window (1200 nm up to 3000 nm) with some potential electrochromic applications related to this spectral window. Light-emitting diodes were fabricated using these copolymers as active layer. To improve hole and electron injection, the active layer was sandwiched between a ITO/PEDOT:PSSA/copolymer/Ba/Al. The emitting properties were studied on the base of photoluminescence (PL) and electroluminescence (EL) expts. The spectral emission varies from blue-green to yellow, depending on the compn. of the copolymers.

IT 174508-31-7P

(monomer; prepn. and optical properties of and LEDs from copolymers prepd. from dibromoethylenedioxythiophene or dibromopyridine and contg. fluorene or phenylene units)

RN 174508-31-7 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro- (9CI) (CA INDEX NAME)



IT 126213-51-2, PEDOT

(prepn. and optical properties of and LEDs from copolymers prepd. from dibromoethylenedioxythiophene or dibromopyridine and contg. fluorene or phenylene units)

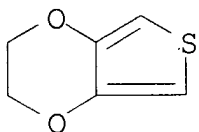
RN 126213-51-2 HCA

CN Thieno[3,4-b]-1,4-dioxin, 2,3-dihydro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 126213-50-1

CMF C6 H6 O2 S



IT 287924-59-8P 287924-60-1P 716377-30-9P
716377-31-0P 716377-32-1P

(prepn. and optical properties of and LEDs from copolymers prepd. from dibromoethylenedioxythiophene or dibromopyridine and contg. fluorene or phenylene units)

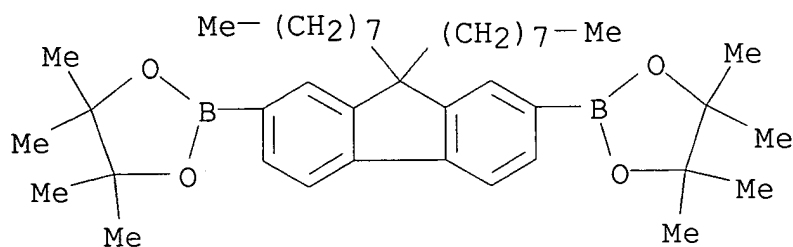
RN 287924-59-8 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro-, polymer with 2,2'-(9,9-dioctyl-9H-fluorene-2,7-diyl)bis[4,4,5,5-tetramethyl-1,3,2-dioxaborolane] (9CI) (CA INDEX NAME)

CM 1

CRN 196207-58-6

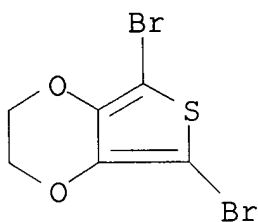
CMF C41 H64 B2 O4



CM 2

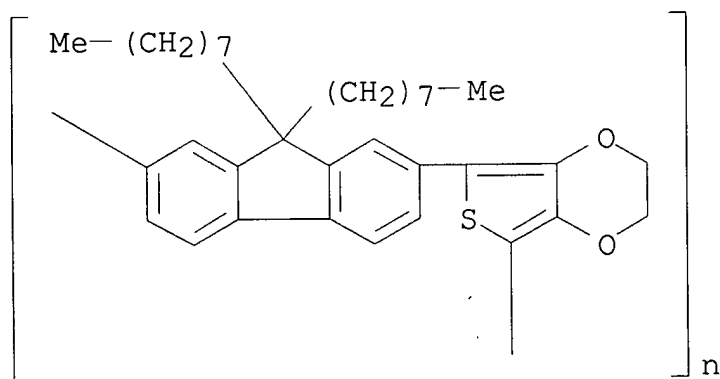
CRN 174508-31-7

CMF C6 H4 Br2 O2 S



RN 287924-60-1 HCA

CN Poly[(2,3-dihydrothieno[3,4-b]-1,4-dioxin-5,7-diyl) (9,9-dioctyl-9H-fluorene-2,7-diyl)] (9CI) (CA INDEX NAME)



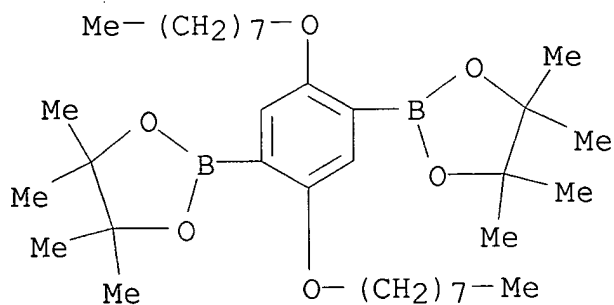
RN 716377-30-9 HCA

CN 1,3,2-Dioxaborolane, 2,2'-[2,5-bis(octyloxy)-1,4-phenylene]bis[4,4,5,5-tetramethyl-, polymer with 5,7-dibromo-2,3-dihydrothieno[3,4-b]-1,4-dioxin (9CI) (CA INDEX NAME)

CM 1

CRN 457931-26-9

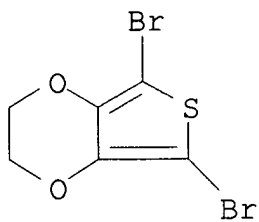
CMF C34 H60 B2 O6



CM 2

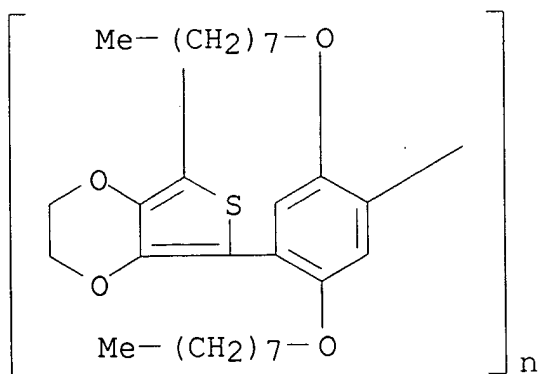
CRN 174508-31-7

CMF C6 H4 Br2 O2 S



RN 716377-31-0 HCA

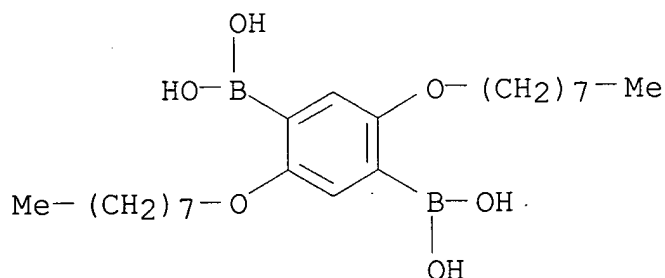
CN Poly[(2,3-dihydrothieno[3,4-b]-1,4-dioxin-5,7-diyl)[2,5-bis(octyloxy)-1,4-phenylene]] (9CI) (CA INDEX NAME)



RN 716377-32-1 HCA
 CN Boronic acid, [2,5-bis(octyloxy)-1,4-phenylene]bis-, polymer with
 5,7-dibromo-2,3-dihydrothieno[3,4-b]-1,4-dioxin (9CI) (CA INDEX
 NAME)

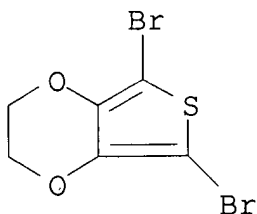
CM 1

CRN 406461-51-6
 CMF C22 H40 B2 O6



CM 2

CRN 174508-31-7
 CMF C6 H4 Br2 O2 S



IT Polymers, preparation
 (conjugated; prepn. and optical properties of and LEDs from
 copolymers prepd. from dibromoethylenedioxythiophene or
 dibromopyridine and contg. fluorene or phenylene units)

IT Doping
 (electrochem.; prepn. and optical properties of and LEDs from
 copolymers prepd. from dibromoethylenedioxythiophene or
 dibromopyridine and contg. fluorene or phenylene units)

IT Conduction electrons
 (injection; prepn. and optical properties of and LEDs from
 copolymers prepd. from dibromoethylenedioxythiophene or
 dibromopyridine and contg. fluorene or phenylene units)

IT Band gap

(optical; prepn. and optical properties of and LEDs from copolymers prepd. from dibromoethylenedioxythiophene or dibromopyridine and contg. fluorene or phenylene units)

- IT Band gap
- Electrochromism
- Electroluminescent devices
- Electronic structure
- Glass substrates
- Glass transition temperature
- HOMO (molecular orbital)
- IR spectra
- LUMO (molecular orbital)
- Luminescence
- Luminescence, electroluminescence
- Polymerization
- Polymerization catalysts
- Raman spectra
- Redox potential
- Redox reaction
- Thermal stability
- UV and visible spectra
- (prepn. and optical properties of and LEDs from copolymers prepd. from dibromoethylenedioxythiophene or dibromopyridine and contg. fluorene or phenylene units)
- IT 9003-53-6D, sulfonated
- (PSS; prepn. and optical properties of and LEDs from copolymers prepd. from dibromoethylenedioxythiophene or dibromopyridine and contg. fluorene or phenylene units)
- IT 7429-90-5, Aluminum, uses 7440-39-3, Barium, uses
- (electrode; prepn. and optical properties of and LEDs from copolymers prepd. from dibromoethylenedioxythiophene or dibromopyridine and contg. fluorene or phenylene units)
- IT 67399-94-4P, 1,4-Dioctyloxybenzene 123863-99-0P,
- 9,9-Dioctylfluorene 156028-40-9P, 1,4-Dibromo-2,5-dioctyloxybenzene 198964-46-4P, 2,7-Dibromo-9,9-dioctylfluorene
- (intermediate in monomer prepn.; prepn. and optical properties of and LEDs from copolymers prepd. from dibromoethylenedioxythiophene or dibromopyridine and contg. fluorene or phenylene units)
- IT 174508-31-7P 196207-58-6P 406461-51-6P 457931-26-9P
- (monomer; prepn. and optical properties of and LEDs from copolymers prepd. from dibromoethylenedioxythiophene or dibromopyridine and contg. fluorene or phenylene units)
- IT 14221-01-3, Pd(PPh₃)₄
- (polymn. catalysts; prepn. and optical properties of and LEDs from copolymers prepd. from dibromoethylenedioxythiophene or dibromopyridine and contg. fluorene or phenylene units)
- IT 50926-11-9, ITO 126213-51-2, PEDOT

(prepn. and optical properties of and LEDs from copolymers prepd. from dibromoethylenedioxythiophene or dibromopyridine and contg. fluorene or phenylene units)

IT 287924-59-8P 287924-60-1P 294637-16-4P
473914-21-5P 633290-76-3P 716377-30-9P
716377-31-0P 716377-32-1P 716377-33-2P
716377-34-3P

(prepn. and optical properties of and LEDs from copolymers prepd. from dibromoethylenedioxythiophene or dibromopyridine and contg. fluorene or phenylene units)

IT 86-73-7, Fluorene 111-83-1, Octyl bromide 123-31-9,
Hydroquinone, reactions 61676-62-8, 2-Isopropoxy-4,4,5,5-
tetramethyl-[1,3,2]dioxaborolane 126213-50-1

(reactant in monomer prepn.; prepn. and optical properties of and LEDs from copolymers prepd. from dibromoethylenedioxythiophene or dibromopyridine and contg. fluorene or phenylene units)

L26 ANSWER 4 OF 29 HCA COPYRIGHT 2005 ACS on STN

141:39122 Synthetic methodology toward new propylenedioxythiophene polymers. Reeves, Benjamin D.; Grenier, Christophe R. G.; Argun, Avni A.; Cirpan, Ali; Cunningham, Garry B.; McCarley, Tracy D.; Reynolds, John R. (Department of Chemistry, Center for Macromolecular Science and Engineering, University of Florida, Gainesville, FL, 32611, USA). Polymer Preprints (American Chemical Society, Division of Polymer Chemistry), 45(1), 284 (English) 2004. CODEN: ACPPAY. ISSN: 0032-3934. Publisher: American Chemical Society, Division of Polymer Chemistry.

AB An extensive family of dioxythiophene-based monomers by Williamson etherification, transesterification, and Mitsunobu chem. has been successfully synthesized by our group, however, the routes developed are not efficient when synthesizing monomers with large substituents. Therefore, a new synthetic methodol. has been employed to access monomers with large nonpolar derivs. First, 3,4-dimethoxythiophene is subject to a transesterification reaction with 2,2-bis(bromomethyl)-1,3-propanediol. The bromomethyl derivatized ProDOT then undergoes a Williamson etherification with octadecanol and the octadecyl deriv. was then brominated with NBS followed by polymn. by Grignard metathesis. The resulting polymer after purifn. by fractionation was characterized by NMR, GPC, MALDI-TOF, X-ray powder diffraction, DSC, and TGA. The polymer was highly sol. in org. solvents, which allowed the spray casting of thin films from soln. and the films were then electrochromically characterized and incorporated into dual polymer electrochromic devices. Also, a polymer soln. in toluene gave a relatively high fluorescence quantum efficiency with a value of 0.40.

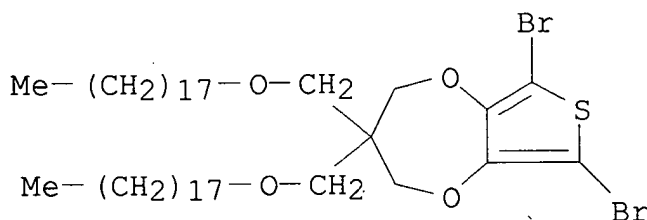
IT 700817-18-1P

(synthesis of propylenedioxythiophene polymers and fluorescence thereof)

RN 700817-18-1 HCA
 CN 2H-Thieno[3,4-b][1,4]dioxepin, 6,8-dibromo-3,4-dihydro-3,3-bis[(octadecyloxy)methyl]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 700817-10-3
 CMF C45 H82 Br2 O4 S



- IT Polymerization
 (Grignard; synthesis of propylenedioxythiophene polymers and fluorescence thereof)
- IT Alkoxylation
 (Williamson; synthesis of propylenedioxythiophene-based monomer for polymers thereof)
- IT Polymerization
 (metathetic; synthesis of propylenedioxythiophene polymers and fluorescence thereof)
- IT Fluorescence
 (of propylenedioxythiophene polymers)
- IT Conducting polymers
 (polythiophenes; synthesis of propylenedioxythiophene polymers and fluorescence thereof)
- IT Etherification
 (transesterification; synthesis of propylenedioxythiophene-based monomer for polymers thereof)
- IT 3296-90-0 51792-34-8
 (in synthesis of propylenedioxythiophene-based monomer for polymers thereof)
- IT 634591-77-8P 701209-98-5P
 (in synthesis of propylenedioxythiophene-based monomer for polymers thereof)
- IT **700817-18-1P**
 (synthesis of propylenedioxythiophene polymers and fluorescence thereof)
- IT 700817-10-3P
 (synthesis of propylenedioxythiophene-based monomer for polymers thereof)

L26 ANSWER 5 OF 29 HCA COPYRIGHT 2005 ACS on STN

141:38937 Processable dioxythiophene based polymers with branched substituents. Grenier, Christophe R. G.; Reeves, Benjamin D.; Argun, Avni A.; Reynolds, John R. (Department of Chemistry, Center for Macromolecular Science and Engineering, University of Florida, Gainesville, FL, 32611, USA). Polymer Preprints (American Chemical Society, Division of Polymer Chemistry), 45(1), 262 (English) 2004. CODEN: ACPPAY. ISSN: 0032-3934. Publisher: American Chemical Society, Division of Polymer Chemistry.

AB We have developed a new family of branched dialkyl and dialkoxy substituted poly(3,4-propylenedioxythiophene)s (PProDOT-R2). Substituents are sym. placed at the 2 position of the propylene bridge. For the monomer synthesis with R=(2-ethylhexyl)oxymethyl and R=(2-methylbutyl)oxymethyl, we used the Williamson etherification on ProDOT-(CH₂Br). For R=2-ethylhexyl, we applied the transesterification technique on 3,4-dimethoxythiophene with the corresponding 2,2-dialkylpropanediol, easily obtained via malonic synthesis followed by redn. with LiAlH₄. The polymer synthesis was carried out using Grignard Metathesis, yielding high mol. wt. polymers (Mn=20,000-50,000 g.mol⁻¹) and dispersities around 1.7. These polymers possess excellent soly. in common org. solvents and allow for easy processability. Spray coated thin films of PProDOT-(CH₂OEtHx) and PProDOT-(EtHx) are electrochromic, switching resp. from absorptive red-purple to a very transmissive light blue color. They exhibit high coloration efficiencies (.apprx.2000 cm²/C) and extremely sharp spectroelectrochem. transitions within a very narrow range of potential (.apprx.0.1V).

IT 700817-14-7P 700817-16-9P

(in prepn. of processable dioxythiophene based polymers with branched substituents)

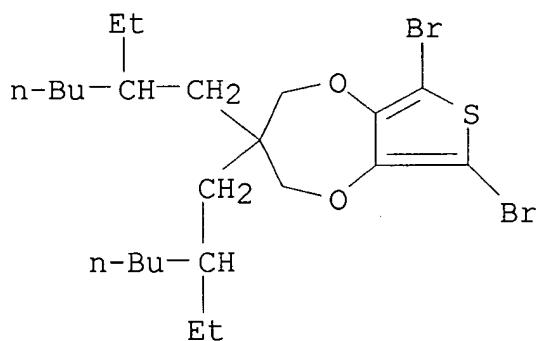
RN 700817-14-7 HCA

CN 2H-Thieno[3,4-b][1,4]dioxepin, 6,8-dibromo-3,3-bis(2-ethylhexyl)-3,4-dihydro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 700817-06-7

CMF C23 H38 Br2 O2 S



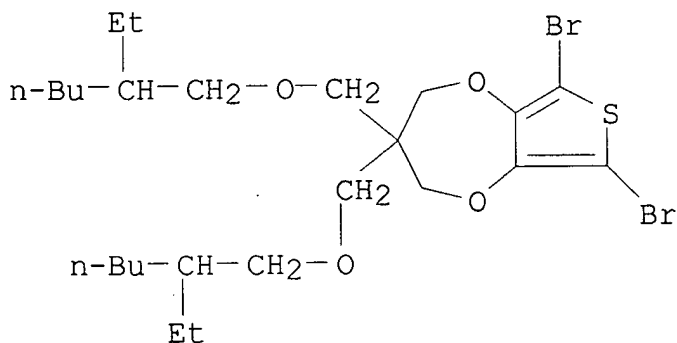
RN 700817-16-9 HCA

CN 2H-Thieno[3,4-b][1,4]dioxepin, 6,8-dibromo-3,3-bis[[2-ethylhexyl]oxy]methyl]-3,4-dihydro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 700817-08-9

CMF C25 H42 Br2 O4 S



- IT Alkylation
 Bromination
 Etherification
 Reduction
 (in prepn. of processable dioxythiophene based polymers with branched substituents)
- IT Polymerization
 (metathetic; in prepn. of processable dioxythiophene based polymers with branched substituents)
- IT Solubility
 (of processable dioxythiophene based polymers with branched substituents)
- IT Conducting polymers

- (polythiophenes; prepn. of processable dioxythiophene based polymers with branched substituents)
- IT Electrochromic materials
(prepn. of processable dioxythiophene based polymers with branched substituents)
- IT Etherification
(transesterification; in prepn. of processable dioxythiophene based polymers with branched substituents)
- IT 700817-14-7P 700817-16-9P
(in prepn. of processable dioxythiophene based polymers with branched substituents)
- IT 104-76-7, 2-Ethylhexanol 105-53-3, Diethyl malonate 18908-66-2, 1-Bromo-2-ethylhexane 51792-34-8, 3,4-Dimethoxythiophene 701209-98-5
(in prepn. of processable dioxythiophene based polymers with branched substituents)
- IT 24251-94-3P 634591-75-6P 700816-90-6P 700817-00-1P
(in prepn. of processable dioxythiophene based polymers with branched substituents)
- L26 ANSWER 6 OF 29 HCA COPYRIGHT 2005 ACS on STN
- 141:24056 Solution processable and electrochromic dioxythiophene-based polymers. Reeves, Benjamin D.; Grenier, Christophe R. G.; Argun, Avni A.; Cirpan, Ali; McCarley, Tracy D.; Reynolds, John R. (Department of Chemistry, Center for Macromolecular Science and Engineering, University of Florida, Gainesville, FL, 32611, USA). Polymer Preprints (American Chemical Society, Division of Polymer Chemistry), 45(1), 180 (English) 2004. CODEN: ACPPAY. ISSN: 0032-3934. Publisher: American Chemical Society, Division of Polymer Chemistry.
- AB This work presents the development of a family of sol. processable disubstituted propylenedioxythiophenes and an anal. of their electrochromic properties. 2,5-Dibromo derivatized dioxythiophene monomers underwent Grignard metathesis polymn. to afford org. sol. neutral polymers. Polymers were characterized by NMR, GPC, MALDI-TOF, X-ray powder diffraction, TGA, and DSC. Mol. wt. characterization by GPC vs. polystyrene stds. indicated no. av. mol. wts. between 7-40 kg/mol. MALDI-TOF studies were performed which gave a set of dominant peaks sepd. by 322 amu, corresponding to the mol. wt. of the monomer repeat unit. Thin films were processed by spray casting polymer solns. onto a working electrode. Spectroelectrochem., colorimetry, and composite coloration efficiencies studies show that the spray cast polymers have the same contrast ratio and switching speeds as the electrodeposited films of the same thickness. The composite coloration efficiency values for this family are two to three times larger than previously obsd. for electrodeposited dioxythiophene polymers.
- IT 700817-12-5P 700817-14-7P 700817-16-9P

700817-18-1P(prepn. of soln. processable and electrochromic
dioxothiophene-based polymers)

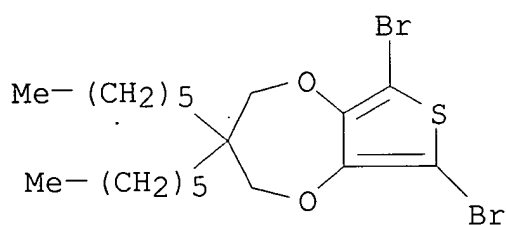
RN 700817-12-5 HCA

CN 2H-Thieno[3,4-b][1,4]dioxepin, 6,8-dibromo-3,3-diethyl-3,4-dihydro-,
homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 700817-04-5

CMF C19 H30 Br2 O2 S



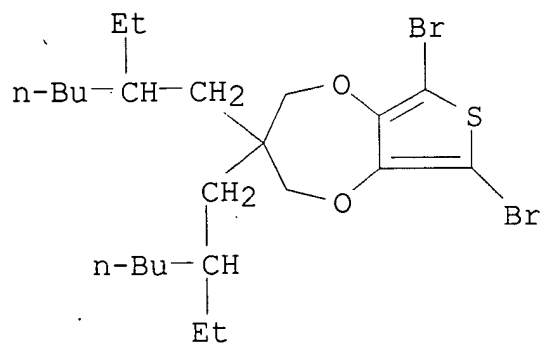
RN 700817-14-7 HCA

CN 2H-Thieno[3,4-b][1,4]dioxepin, 6,8-dibromo-3,3-bis(2-ethylhexyl)-3,4-
dihydro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 700817-06-7

CMF C23 H38 Br2 O2 S



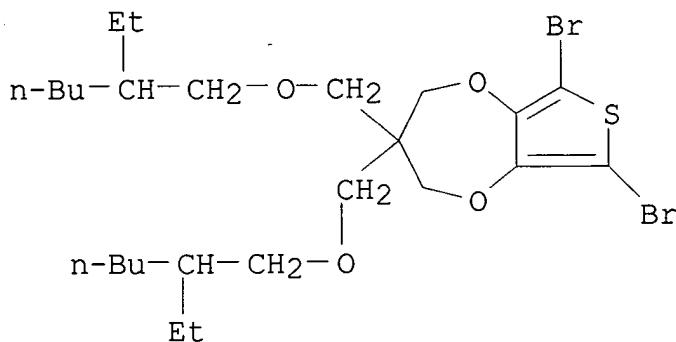
RN 700817-16-9 HCA

CN 2H-Thieno[3,4-b][1,4]dioxepin, 6,8-dibromo-3,3-bis[[2-
ethylhexyl)oxy)methyl]-3,4-dihydro-, homopolymer (9CI) (CA INDEX
NAME)

CM 1

CRN 700817-08-9

CMF C25 H42 Br2 O4 S



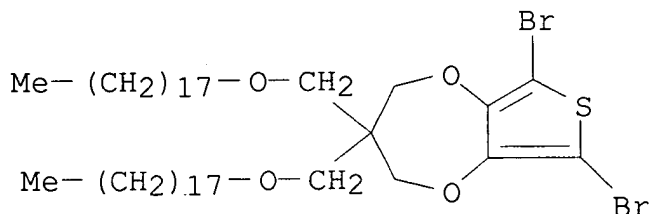
RN 700817-18-1 HCA

CN 2H-Thieno[3,4-b][1,4]dioxepin, 6,8-dibromo-3,4-dihydro-3,3-bis[(octadecyloxy)methyl]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 700817-10-3

CMF C45 H82 Br2 O4 S



IT Alkoxylation

(Williamson; in prepn. of monomers for soln. processable and electrochromic dioxothiophene-based polymers)

IT Bromination

Transesterification

(in prepn. of monomers for soln. processable and electrochromic dioxothiophene-based polymers)

IT Polymerization

(metathetic; in prepn. of soln. processable and electrochromic dioxothiophene-based polymers)

IT Optical switching

(of electrochromic dioxothiophene-based polymers)

IT Molecular weight

(of soln. processable and electrochromic dioxothiophene-based

- polymers)
- IT Conducting polymers
(polythiophenes; prepn. of soln. processable and electrochromic dioxithiophene-based polymers)
- IT Electrochromic materials
(prepn. of soln. processable and dioxithiophene-based polymers for electrochromic materials)
- IT 128-08-5, N-Bromosuccinimide
(in prepn. of monomers for soln. processable and electrochromic dioxithiophene-based polymers)
- IT 51792-34-8, 3,4-Dimethoxythiophene 54662-33-8 57355-20-1
700816-90-6 700816-93-9
(in prepn. of soln. processable and electrochromic dioxithiophene-based polymers)
- IT 634591-75-6P 634591-77-8P 700816-98-4P 700817-00-1P
(in prepn. of soln. processable and electrochromic dioxithiophene-based polymers)
- IT 700817-04-5P 700817-06-7P 700817-08-9P 700817-10-3P
(monomer; in prepn. of soln. processable and electrochromic dioxithiophene-based polymers)
- IT 700817-12-5P 700817-14-7P 700817-16-9P
700817-18-1P
(prepn. of soln. processable and electrochromic dioxithiophene-based polymers)

L26 ANSWER 7 OF 29 HCA COPYRIGHT 2005 ACS on STN

140:77531 Solid-State Synthesis of a Conducting Polythiophene via an Unprecedented Heterocyclic Coupling Reaction. Meng, Hong; Perepichka, Dmitrii F.; Bendikov, Michael; Wudl, Fred; Pan, Grant Z.; Yu, Wenjiang; Dong, Wenjian; Brown, Stuart (Department of Chemistry and Biochemistry and the Exotic Materials Institute, Microfabrication Lab, Department of Physics and Astrophysics, University of California, Los Angeles, CA, 90095-1569, USA). Journal of the American Chemical Society, 125(49), 15151-15162 (English) 2003. CODEN: JACSAT. ISSN: 0002-7863. Publisher: American Chemical Society.

AB Prolonged storage (.apprx.2 yr) or gentle heating (50-80 °C) of cryst. 2,5-dibromo-3,4-ethylenedioxythiophene (DBEDOT) affords a highly conducting, bromine-doped poly(3,4-ethylenedioxythiophene) (PEDOT), as confirmed by solid-state NMR, FTIR, CV, and vis-NIR spectroscopies. The novel solid-state polymn. (SSP) does not occur for 2,5-dichloro-3,4-ethylenedioxythiophene (DCEDOT), and requires a much higher temp. (>130 °C) for 2,5-diiodo-3,4-ethylenedioxythiophene (DIEDOT). X-ray structural anal. of the above dihalothiophenes reveals short Hal...Hal distances between adjacent mols. in DBEDOT and DIEDOT, but not in DCEDOT. The polymn. may also occur in the melt but is significantly slower and leads to poorly conductive material. Detailed studies of

the reaction were performed using ESR, DSC, microscopy, and gravimetric analyses. SSP starts on crystal defect sites; it is exothermic by 14 kcal/mol and requires activation energy of .apprx.26 kcal/mol (for DBEDOT). The temp. dependence of the cond. of SSP-PEDOT (σ_{rt} = 20-80 S/cm) reveals a slight thermal activation. It can be further increased by a factor of 2 by doping with iodine. Using this approach, thin films of PEDOT with cond. as high as 20 S/cm were fabricated on insulating flexible plastic surfaces.

IT **350037-71-7P**, 2,5-Dibromo-3,4-Ethylenedioxythiophene homopolymer

(solid-state synthesis of conducting polythiophenes via unprecedented heterocyclic coupling reaction)

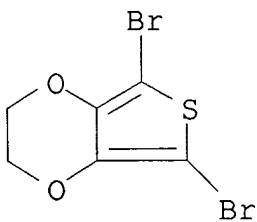
RN 350037-71-7 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 174508-31-7

CMF C6 H4 Br2 O2 S



IT NMR spectroscopy
(carbon-13, solid state; solid-state synthesis of conducting polythiophenes via unprecedented heterocyclic coupling reaction)

IT Polymer morphology
(cryst.; solid-state synthesis of conducting polythiophenes via unprecedented heterocyclic coupling reaction)

IT Conducting polymers
(polythiophenes; solid-state synthesis of conducting polythiophenes via unprecedented heterocyclic coupling reaction)

IT Electric conductivity
(solid-state synthesis of conducting polythiophenes via unprecedented heterocyclic coupling reaction)

IT 225518-49-0P, 2,5-Dichloro-3,4-Ethylenedioxythiophene 640737-72-0P
(solid-state synthesis of conducting polythiophenes via unprecedented heterocyclic coupling reaction)

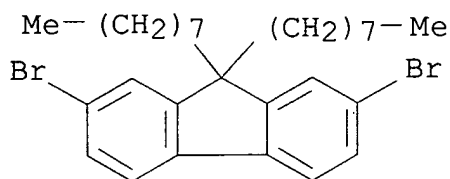
IT **350037-71-7P**, 2,5-Dibromo-3,4-Ethylenedioxythiophene homopolymer

- (solid-state synthesis of conducting polythiophenes via unprecedented heterocyclic coupling reaction)
- IT 174508-31-7P, 2,5-Dibromo-3,4-Ethylenedioxythiophene . 640737-73-1P
(solid-state synthesis of conducting polythiophenes via unprecedented heterocyclic coupling reaction)
- IT 109-72-8, n-Butyl lithium, reactions 128-08-5, N-Bromosuccinimide
128-09-6, N-Chlorosuccinimide 1600-27-7, Mercuric acetate
7553-56-2, Iodine, reactions 126213-50-1, 3,4-Ethylenedioxythiophene
(solid-state synthesis of conducting polythiophenes via unprecedented heterocyclic coupling reaction)
- L26 ANSWER 8 OF 29 HCA COPYRIGHT 2005 ACS on STN
- 139:133926 Synthesis and electroluminescent properties of copolymers derived from fluorene and thiophene derivatives. Hou, Q.; Niu, Y. H.; Huang, W. B.; Yang, W.; Yang, R. Q.; Yuan, M.; Cao, Y. (Institute of Polymer Optoelectronic Materials and Devices, South China University of Technology, Canton, 510640, Peop. Rep. China). Synthetic Metals, 135-136, 185-186 (English) 2003. CODEN: SYMEDZ. ISSN: 0379-6779. Publisher: Elsevier Science B.V..
- AB A series of sol. conjugated polymers of 2,7-dibromo-9,9-dioctylfluorene, 2,7-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-9,9-dioctylfluorene (DOF)s with thiophene (TOP) or 2,5-dibromo-3,4-ethylenedioxythiophene (EDT) were synthesized via palladium-catalyzed Suzuki coupling reaction. The DOFs-EDT and DOFs-TOP copolymers have comonomer ratio that is very close to the feed ratio, have alternating DOF monomer units, and give rise to various emission colors from bluish-green to yellow. The highest electroluminescence (EL) quantum efficiency the copolymers is 1.8% for DOFs-EDT and 0.45% for DOFs-TOP, as measured in test device of ITO/polythiophene-polyfluorene/Ba/Al structure. The enhanced quantum efficiency is of interest for application in PLED displays.
- IT 569355-28-8P, 2,7-Bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-9,9-dioctylfluorene-2,5-dibromo-3,4-ethylenedioxythiophene-2,7-dibromo-9,9-dioctylfluorene copolymer
(prepn. of sol. conjugated polythiophene-polyfluorenes with high electroluminescence quantum efficiency)
- RN 569355-28-8 HCA
- CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro-, polymer with 2,7-dibromo-9,9-dioctyl-9H-fluorene and 2,2'-(9,9-dioctyl-9H-fluorene-2,7-diyl)bis[4,4,5,5-tetramethyl-1,3,2-dioxaborolane] (9CI)
(CA INDEX NAME)

CM 1

CRN 198964-46-4

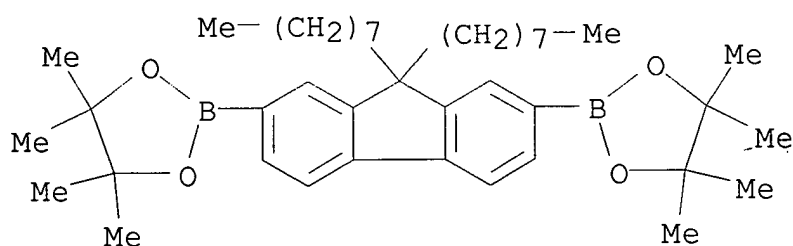
CMF C29 H40 Br2



CM 2

CRN 196207-58-6

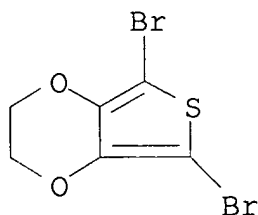
CMF C41 H64 B2 O4



CM 3

CRN 174508-31-7

CMF C6 H4 Br2 O2 S



- IT Polymerization
 (Suzuki coupling; prepn. of sol. conjugated polythiophene-
 polyfluorenes with high electroluminescence quantum efficiency)
- IT Polymers, preparation
 (conjugated; prepn. of sol. conjugated polythiophene-
 polyfluorenes with high electroluminescence quantum efficiency)
- IT Conducting polymers
 (polythiophenes; prepn. of sol. conjugated polythiophene-
 polyfluorenes with high electroluminescence quantum efficiency)
- IT Luminescence, electroluminescence
 Optical absorption

Solubility

Suzuki coupling reaction

(prepn. of sol. conjugated polythiophene-polyfluorenes with high electroluminescence quantum efficiency)

IT 569355-28-8P, 2,7-Bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-9,9-dioctylfluorene-2,5-dibromo-3,4-ethylenedioxythiophene-2,7-dibromo-9,9-dioctylfluorene copolymer 569355-29-9P, 2,7-Bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-9,9-dioctylfluorene-2,7-dibromo-9,9-dioctylfluorene-2,5-dibromothiophene copolymer

(prepn. of sol. conjugated polythiophene-polyfluorenes with high electroluminescence quantum efficiency)

L26 ANSWER 9 OF 29 HCA COPYRIGHT 2005 ACS on STN

139:53566 Electronic and optical properties of polyfluorene and fluorene-based copolymers: a quantum-chemical characterization. Cornil, J.; Gueli, I.; Dkhissi, A.; Sancho-Garcia, J. C.; Hennebicq, E.; Calbert, J. P.; Lemaure, V.; Beljonne, D.; Bredas, J. L. (Center for Research in Molecular Electronics and Photonics, Laboratory for Chemistry of Novel Materials, University of Mons-Hainaut, Mons, B-7000, Belg.). Journal of Chemical Physics, 118(14), 6615-6623 (English) 2003. CODEN: JCPSA6. ISSN: 0021-9606. Publisher: American Institute of Physics.

AB A detailed quantum-chem. study was carried out of the electronic and optical properties of polyfluorene chains vs. those in copolymers contg. alternating fluorene and benzothiadiazole or ethylenedioxythiophene units. The comonomer has an important role on the excitonic properties and the efficiency of charge- and energy-transfer processes. The choice of comonomer is thus crit. in targeting specific optical properties while maintaining good carrier transport properties in polyfluorenes.

IT 498358-35-3
(quantum chem. study of electronic excitation and optical band gap of polyfluorene and fluorene-based copolymers)

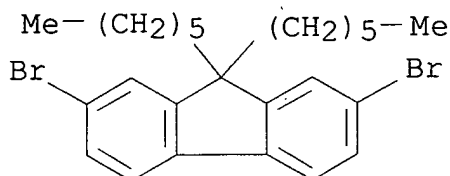
RN 498358-35-3 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro-, polymer with 2,7-dibromo-9,9-dihexyl-9H-fluorene (9CI) (CA INDEX NAME)

CM 1

CRN 189367-54-2

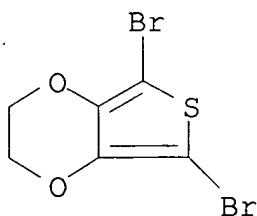
CMF C25 H32 Br2



CM 2

CRN 174508-31-7

CMF C6 H4 Br2 O2 S



- IT Polymers, properties
(conjugated; quantum chem. study of electronic excitation and optical band gap of polyfluorene and fluorene-based copolymers)
- IT Conducting polymers
(polythiophenes, ethylenedioxythiophene and benzothiadiazole, polyfluorenes; quantum chem. study of electronic excitation and optical band gap of polyfluorene and fluorene-based copolymers)
- IT Band structure
Electronic energy transfer
Excited state
Exciton
HOMO (molecular orbital)
LUMO (molecular orbital)
Triplet state
(quantum chem. study of electronic excitation and optical band gap of polyfluorene and fluorene-based copolymers)
- IT 123864-00-6 210347-52-7 **498358-35-3**
(quantum chem. study of electronic excitation and optical band gap of polyfluorene and fluorene-based copolymers)

L26 ANSWER 10 OF 29 HCA COPYRIGHT 2005 ACS on STN
139:7558 New fluorene-based light-emitting copolymers. Cao, Yong; Hou, Qiong; Niu, Yu-hua; Yang, Ren-qiang; Xu, Yi-she; Luo, Jie; Yang, Wei (Institute of Polymer Optoelectronic Materials and Devices, South China Univ. of Tech., Canton, 510640, Peop. Rep. China). Huanan

Ligong Daxue Xuebao, Ziran Kexueban, 30(11), 1-10 (Chinese) 2002.
CODEN: HLDKEZ. ISSN: 1000-565X. Publisher: Huanan Ligong Daxue
Xuebao Bianji Weiyuanhui.

AB A series of novel random copolymers based on 9,9-dioctylfluorene (DOF) and thiophene or its derivs. (ethylenedioxythiophene (EDT), 4,7-dithien-2-yl-2,1,3-benzo thiadiazole (DBT), 4,7-dithien-2-yl-2,1,3-benzoselenadiazole(BTSe)) were synthesized by the palladium-catalyzed Suzuki coupling method. The successful color tuning from green (490 .apprx. 560 nm) to red (628 .apprx. 718 nm) was obtained. The PL and EL quantum efficiencies of these random copolymers are higher than those of alternating copolymers reported by other researchers. The maximal EL quantum efficiency is 0.45% for copolymer of fluorene and thiophene, 1.8% for copolymer of fluorene and EDT, 1.4% for copolymer of fluorene and DBT and 0.5% for copolymers of fluorene and BTSe. This is the highest EL external efficiency reported so far for the same fluorene-based copolymers. The efficient energy transfer due to exciton trapping on the narrow band-gap BTSe or DBT sites has been obsd. The results indicate that the use of conjugated polyfluorene as wide band-gap segment with a small amt. of narrow band-gap dopant in the polymer main chain could provide a new way to combine high quantum efficiency along with color tuning ability.

IT 287924-59-8

(fluorene-based light-emitting copolymers)

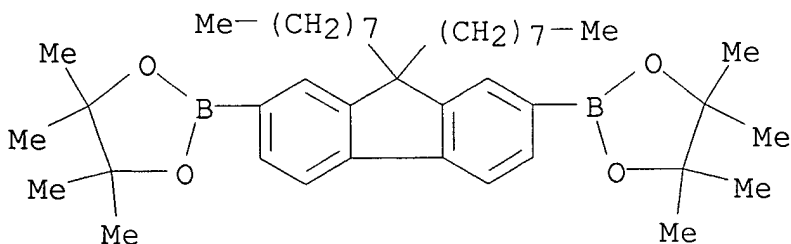
RN 287924-59-8 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro-, polymer with 2,2'-(9,9-dioctyl-9H-fluorene-2,7-diyl)bis[4,4,5,5-tetramethyl-1,3,2-dioxaborolane] (9CI) (CA INDEX NAME)

CM 1

CRN 196207-58-6

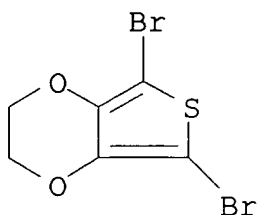
CMF C41 H64 B2 O4



CM 2

CRN 174508-31-7

CMF C6 H4 Br2 O2 S



IT HOMO (molecular orbital)

LUMO (molecular orbital)

Luminescence

Oxidation potential

(fluorene-based light-emitting copolymers)

IT 222857-62-7 **287924-59-8** 534591-71-4 534591-73-6

(fluorene-based light-emitting copolymers)

L26 ANSWER 11 OF 29 HCA COPYRIGHT 2005 ACS on STN

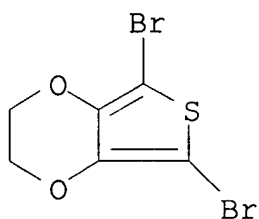
138:304877 3,4-Ethylenedioxy-substituted bithiophene-alt-thiophene-S,S-dioxide regular copolymers. Synthesis and conductive, magnetic and luminescence properties.. Berlin, Anna; Zotti, Gianni; Zecchin, Sandro; Schiavon, Gilberto; Cocchi, Massimo; Virgili, Dalia; Sabatini, Cristiana (Istituto CNR di Scienze e Tecnologie Molecolari, Milan, 20133, Italy). Journal of Materials Chemistry, 13(1), 27-33 (English) 2003. CODEN: JMACEP. ISSN: 0959-9428. Publisher: Royal Society of Chemistry.

AB Polyconjugated regular bithiophene-alt-thiophene-S,S-dioxide copolymers were produced by anodic coupling of variously 3,4-ethylenedioxy-substituted 2,5-bis(2-thienyl)thiophene-S,S-dioxide. The polymers were characterized by cyclic voltammetry, FTIR reflection-absorption and UV-vis spectroscopy, MALDI-TOF mass spectroscopy, electrochem. quartz crystal microbalance, in situ ESR and in situ cond. techniques, photo- and electro-luminescence measurements. The regular alternation of electron-rich and -poor thiophene rings in the polymer chain operated by the ethylenedioxy and S,S-dioxide moieties produces a finite window of cond. Alkyl-protection of the β -positions of the thiophene-S,S-dioxide ring gave low-defect and sol. oligomers which were investigated in single-layer org. light-emitting devices (OLEDs). Photoluminescence quantum efficiency of .apprx.1% and external electroluminescence quantum efficiencies of 0.01% photon/electron at a luminance of 100 cd m⁻² were obtained.

IT **174508-31-7**, 2,5-Dibromo-3,4-(ethylenedioxy)thiophene
(oxidn. of)

RN 174508-31-7 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro- (9CI) (CA INDEX NAME)



IT 511286-88-7P 511286-89-8P 511286-90-1P
511286-91-2P 511286-92-3P

(prepn. and conductive, magnetic and luminescence properties of)

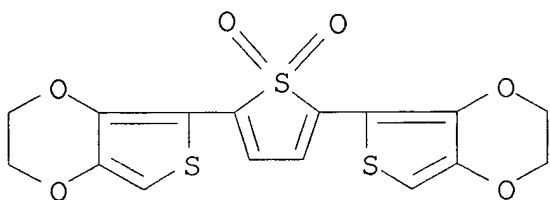
RN 511286-88-7 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,5'-(1,1-dioxido-2,5-thiophenediyl)bis[2,3-dihydro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 511286-81-0

CMF C16 H12 O6 S3



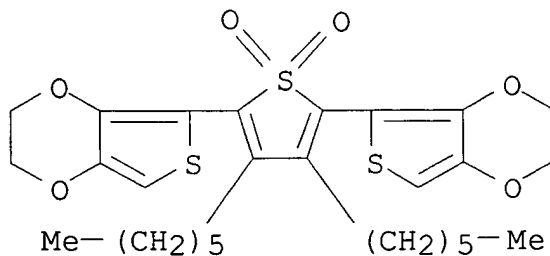
RN 511286-89-8 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,5'-(3,4-dihexyl-1,1-dioxido-2,5-thiophenediyl)bis[2,3-dihydro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 511286-82-1

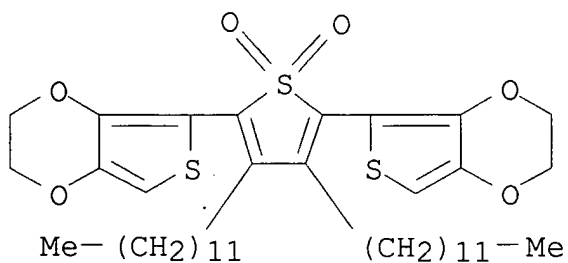
CMF C28 H36 O6 S3



RN 511286-90-1 HCA
CN Thieno[3,4-b]-1,4-dioxin, 5,5'-(3,4-didodecyl-1,1-dioxido-2,5-thiophenediyl)bis[2,3-dihydro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

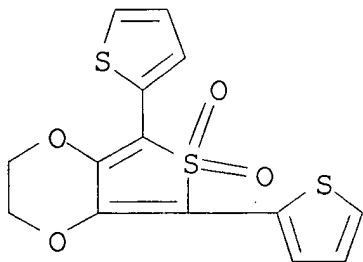
CRN 511286-83-2
CMF C40 H60 O6 S3



RN 511286-91-2 HCA
CN Thieno[3,4-b]-1,4-dioxin, 2,3-dihydro-5,7-di-2-thienyl-, 6,6-dioxide, homopolymer (9CI) (CA INDEX NAME)

CM 1

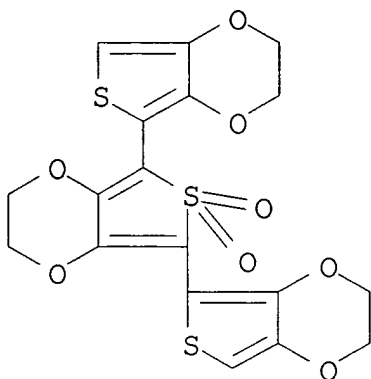
CRN 511286-84-3
CMF C14 H10 O4 S3



RN 511286-92-3 HCA
CN 5,5':7',5''-Terthieno[3,4-b]-1,4-dioxin, 2,2',2'',3,3',3''-hexahydro-, 6',6'-dioxide, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 511286-85-4
CMF C18 H14 O8 S3

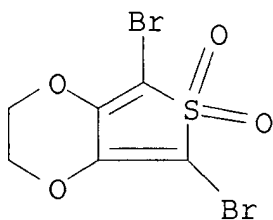


IT 511286-87-6P

(prepn. and reaction with (tributylstannyl)thiophene)

RN 511286-87-6 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro-, 6,6-dioxide
(9CI) (CA INDEX NAME)



IT Oxidation potential

Reduction potential

(of ethylenedioxy-substituted bis(thienyl)thiophene dioxide
monomers and polymers)

IT Electric conductivity

Luminescence

Luminescence, electroluminescence

(prepn. and conductive, magnetic and luminescence properties of
ethylenedioxy-substituted bithiophene-alt-thiophene dioxide
polymers)

IT Electroluminescent devices

(single-layer electroluminescence devices prepd. from
ethylenedioxy-substituted bithiophene-alt-thiophene dioxide
polymers)

IT Polycarbonates, properties

(single-layer electroluminescence devices prepd. from
ethylenedioxy-substituted bithiophene-alt-thiophene dioxide
polymers and)

IT 25037-45-0, Bisphenol A polycarbonate

(assumed monomers; single-layer electroluminescence devices)

- prepd. from ethylenedioxy-substituted bithiophene-alt-thiophene dioxide polymers and)
- IT 174508-31-7, 2,5-Dibromo-3,4-(ethylenedioxy)thiophene
174509-52-5
(oxidn. of)
- IT 511286-88-7P 511286-89-8P 511286-90-1P
511286-91-2P 511286-92-3P
(prepn. and conductive, magnetic and luminescence properties of)
- IT 511286-81-0P 511286-82-1P 511286-83-2P 511286-84-3P
511286-85-4P
(prepn. and polymn. of)
- IT 511286-86-5P
(prepn. and reaction with (tributylstannyl)(ethylenedioxy)thiophene)
- IT 511286-87-6P
(prepn. and reaction with (tributylstannyl)thiophene)
- IT 89088-95-9, 2,5-Dibromothiophene-1,1-dioxide
(reaction with (tributylstannyl)(ethylenedioxy)thiophene)
- IT 175922-79-9, 2-(Tributylstannyl)-3,4-(ethylenedioxy)thiophene
(reaction with dibromothiophene dioxide)
- IT 24936-68-3, Bisphenol A polycarbonate, sru, properties 65181-78-4,
N,N'-Diphenyl-N,N'-bis(3-methylphenyl)-1,1'-biphenyl-4,4'-diamine
(single-layer electroluminescence devices prepd. from
ethylenedioxy-substituted bithiophene-alt-thiophene dioxide
polymers and)

L26 ANSWER 12 OF 29 HCA COPYRIGHT 2005 ACS on STN

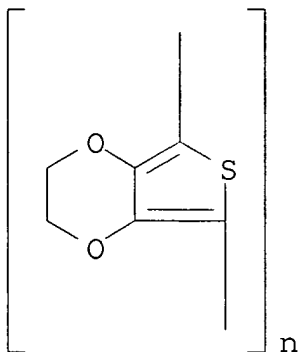
138:288055 Facile solid-state synthesis of highly conducting poly(ethylenedioxythiophene). Meng, Hong; Perepichka, Dmitrii F.; Wudl, Fred (Department of Chemistry and Biochemistry and Exotic Materials Institute, University of California, Los Angeles, CA, 90095-1569, USA). Angewandte Chemie, International Edition, 42(6), 658-661 (English) 2003. CODEN: ACIEF5. ISSN: 1433-7851. Publisher: Wiley-VCH Verlag GmbH & Co. KGaA.

AB The prepn. of PEDOT by catalyst-free coupling polymn. of 2,5-dibromo-3,4-ethylenedioxythiophene in the solid state at accelerated temps. (60, 80, and 120°) is reported. The cond. of polymer films on plastic and glass substrate was examd. Crystal structure data for the monomer are presented.

IT 163359-60-2P, 2,5-Dibromo-3,4-ethylenedioxythiophene homopolymer, SRU 350037-71-7P, 2,5-Dibromo-3,4-ethylenedioxythiophene homopolymer
(solid-state polymn. of dibromoethylenedioxythiophene and cond. of poly(ethylenedioxythiophene))

RN 163359-60-2 HCA

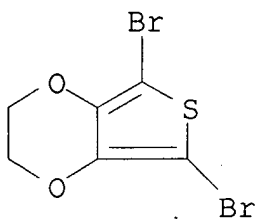
CN Poly(2,3-dihydrothieno[3,4-b]-1,4-dioxin-5,7-diyl) (9CI) (CA INDEX NAME)



RN 350037-71-7 HCA
 CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro-, homopolymer
 (9CI) (CA INDEX NAME)

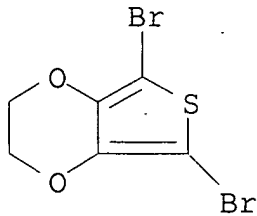
CM 1

CRN 174508-31-7
 CMF C6 H4 Br2 O2 S



IT 174508-31-7, 2,5-Dibromo-3,4-ethylenedioxythiophene
 (structure and solid-state polymn. of
 dibromoethylenedioxythiophene)

RN 174508-31-7 HCA
 CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro- (9CI) (CA INDEX
 NAME)



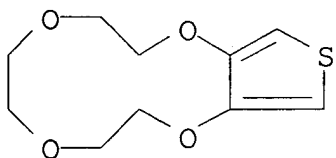
IT Polymer morphology

- (cryst.; solid-state polymn. of dibromoethylenedioxythiophene and cond. of poly(ethylenedioxythiophene))
- IT Crystal structure
(of 2,5-dibromo-3,4-ethylenedioxythiophene)
- IT Conducting polymers
Electric conductivity
(solid-state polymn. of dibromoethylenedioxythiophene and cond. of poly(ethylenedioxythiophene))
- IT **163359-60-2P**, 2,5-Dibromo-3,4-ethylenedioxythiophene homopolymer, **SRU 350037-71-7P**, 2,5-Dibromo-3,4-ethylenedioxythiophene homopolymer
(solid-state polymn. of dibromoethylenedioxythiophene and cond. of poly(ethylenedioxythiophene))
- IT **174508-31-7**, 2,5-Dibromo-3,4-ethylenedioxythiophene
(structure and solid-state polymn. of dibromoethylenedioxythiophene)
- L26 ANSWER 13 OF 29 HCA COPYRIGHT 2005 ACS on STN
- 138:188206 EQCM analysis of the alkali metal ion coordination properties of novel poly(thiophene)s 3,4-functionalized with crown-ether moieties. Berlin, A.; Zotti, G.; Zecchin, S.; Schiavon, G. (Istituto CNR di Scienze e Tecnologie Molecolari, Milan, 20133, Italy). Synthetic Metals, 131(1-3), 149-160 (English) 2002. CODEN: SYMEDZ. ISSN: 0379-6779. Publisher: Elsevier Science B.V..
- AB New thiophenes carrying 18-crown-6-ether ring directly linked to the 3- and 4-positions of the thiophene ring were synthesized and polymd. by anodic coupling in acetonitrile. The polymers were characterized by cyclic voltammetry (CV), UV-Vis and FTIR spectroscopy, matrix-assisted laser desorption ionization (MALDI) mass spectroscopy and in situ cond. Electrochem. quartz crystal microbalance (EQCM) anal. of the alkali metal coordination ability of the 18-crown-6-ether polymer films in acetonitrile has evidenced that the coordination consts. (e.g. 20-80 M⁻¹ for Na⁺) are ca. two orders of magnitude lower than those of polythiophenes bearing the crown substituents pendant from the polythiophene backbone. The result has been ascribed both to electronic and solid-state effects of the conjugated polythiophene chains.
- IT **249513-23-3P 484640-50-8P 484640-51-9P 497937-33-4P 497937-34-5P**
(EQCM anal. of alkali metal ion coordination properties of poly(thiophene)s 3,4-functionalized with crown-ether moieties)
- RN 249513-23-3 HCA
- CN Thieno[3,4-b]-1,4,7,10-tetraoxacyclododecin, 2,3,5,6,8,9-hexahydro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 122372-73-0

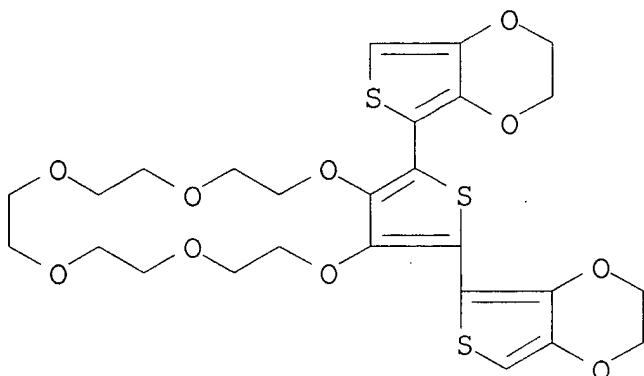
CMF C10 H14 O4 S



RN 484640-50-8 HCA
 CN Thieno[3,4-b]-1,4,7,10,13,16-hexaoxacyclooctadecin,
 17,19-bis(2,3-dihydrothieno[3,4-b]-1,4-dioxin-5-yl)-
 2,3,5,6,8,9,11,12,14,15-decahydro-, homopolymer (9CI) (CA INDEX
 NAME)

CM 1

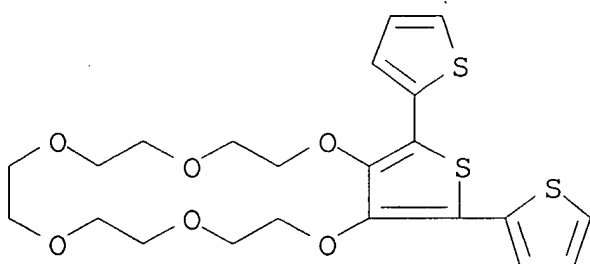
CRN 484640-48-4
 CMF C26 H30 O10 S3



RN 484640-51-9 HCA
 CN Thieno[3,4-b]-1,4,7,10,13,16-hexaoxacyclooctadecin,
 2,3,5,6,8,9,11,12,14,15-decahydro-17,19-di-2-thienyl-, homopolymer
 (9CI) (CA INDEX NAME)

CM 1

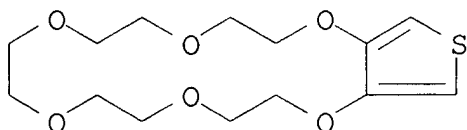
CRN 484640-49-5
 CMF C22 H26 O6 S3



RN 497937-33-4 HCA
 CN Thieno[3,4-b]-1,4,7,10,13,16-hexaoxacyclooctadecin,
 2,3,5,6,8,9,11,12,14,15-decahydro-, homopolymer (9CI) (CA INDEX
 NAME)

CM 1

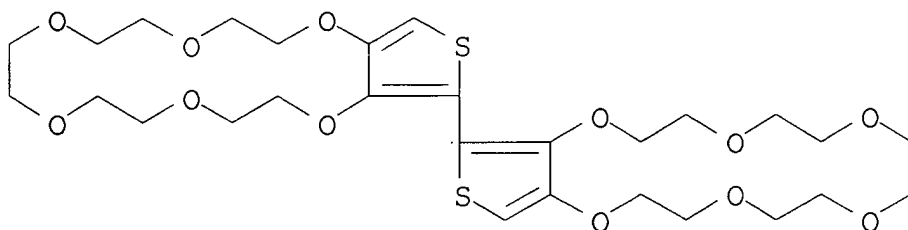
CRN 122372-75-2
 CMF C14 H22 O6 S



RN 497937-34-5 HCA
 CN 17,17'-Bithieno[3,4-b]-1,4,7,10,13,16-hexaoxacyclooctadecin,
 2,2',3,3',5,5',6,6',8,8',9,9',11,11',12,12',14,14',15,15'-
 eicosahydro-, homopolymer (9CI) (CA INDEX NAME)

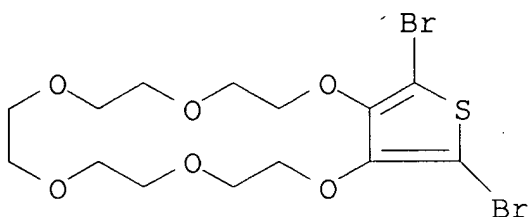
CM 1

CRN 497937-32-3
 CMF C28 H42 O12 S2



IT 233756-39-3P
 (EQCM anal. of alkali metal ion coordination properties of

poly(thiophene)s 3,4-functionalized with crown-ether moieties)
 RN 233756-39-3 HCA
 CN Thieno[3,4-b]-1,4,7,10,13,16-hexaoxacyclooctadecin,
 17,19-dibromo-2,3,5,6,8,9,11,12,14,15-decahydro- (9CI) (CA INDEX
 NAME)



IT Cyclic voltammetry
 Electric conductivity
 (EQCM anal. of alkali metal ion coordination properties of
 poly(thiophene)s 3,4-functionalized with crown-ether moieties)
 IT Polymerization
 (electrochem.; EQCM anal. of alkali metal ion coordination
 properties of poly(thiophene)s 3,4-functionalized with
 crown-ether moieties)
 IT 7439-93-2, Lithium, properties 7440-23-5, Sodium, properties
 (EQCM anal. of alkali metal ion coordination properties of
 poly(thiophene)s 3,4-functionalized with crown-ether moieties)
 IT 249513-23-3P 484640-50-8P 484640-51-9P
 497937-33-4P 497937-34-5P
 (EQCM anal. of alkali metal ion coordination properties of
 poly(thiophene)s 3,4-functionalized with crown-ether moieties)
 IT 122372-75-2 126213-50-1 484640-48-4 484640-49-5
 (EQCM anal. of alkali metal ion coordination properties of
 poly(thiophene)s 3,4-functionalized with crown-ether moieties)
 IT 233756-39-3P 497937-32-3P
 (EQCM anal. of alkali metal ion coordination properties of
 poly(thiophene)s 3,4-functionalized with crown-ether moieties)

L26 ANSWER 14 OF 29 HCA COPYRIGHT 2005 ACS on STN

138:188177 New organic materials for light emitting devices based on
 dihexyl-fluorene-co-ethylenedioxythiophene copolymers exhibiting
 improved hole-injecting properties. Stephan, Olivier; Tran-Van,
 Francois; Chevrot, Claude (Universite Joseph Fourier Grenoble 1 and
 CNRS (UMR C5588), Laboratoire de Spectrometrie Physique, Saint
 Martin d'Heres, 38402, Fr.). Synthetic Metals, 131(1-3), 31-40
 (English) 2002. CODEN: SYMEDZ. ISSN: 0379-6779. Publisher:
 Elsevier Science B.V..

AB We report the synthesis, optical and electrochem. characterizations
 of 9,9-di-n-hexyl-fluorene-co-3,4-ethylenedioxythiophene

(DHF-co-EDOT) copolymers obtained from a mixt., in various ratios, of the two corresponding di-brominated monomers by dehalogenation polycondensation. Elemental anal., IR studies coupled with ¹H NMR clearly indicate, as expected, that the amt. of each monomer unit in the final materials is strongly correlated with the feed compn. even though the reactivity of the di-brominated EDOT seems lower than that of di-brominated DHF. It appears that even a low EDOT content, i.e. 11-15 mol%, within a PDHF main chain, leading to the copolymer COP01, caused significant changes in the electronic properties of the material when compared to PDHF homopolymer. Higher EDOT contents lead to less sol. copolymers which are not suitable for investigation of their use as luminescent semiconducting π -conjugated materials in org. light emitting diodes. Green org. light emitting devices based on COP01 have been investigated and showed improved hole injection properties when compared to devices based on PDHF homopolymer. The origin of the emitted light has been attributed to the concomitant emission of aggregates PDHF segments with EDOT short oligomeric segments. The use of an addnl. poly(3,4-ethylenedioxythiophene-2,5-diyl) -polystyrene sulfonate layer on the indium tin oxide (ITO) anode has also been investigated and leads to improved operating lifetime.

IT 350037-71-7, 2,5-Dibromo-3,4-ethylenedioxythiophene homopolymer

(improved hole-injecting properties of copolymers dihexylfluorene with ethylenedioxythiophene)

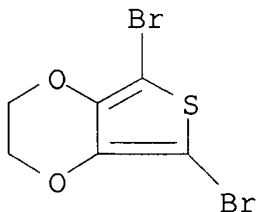
RN 350037-71-7 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 174508-31-7

CMF C6 H4 Br2 O2 S



IT 498358-35-3P

(improved hole-injecting properties of copolymers dihexylfluorene with ethylenedioxythiophene)

RN 498358-35-3 HCA

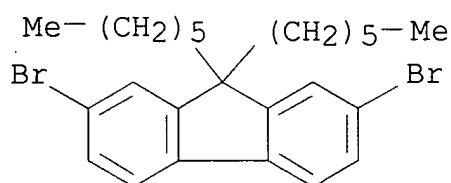
CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro-, polymer with

2,7-dibromo-9,9-dihexyl-9H-fluorene (9CI) (CA INDEX NAME)

CM 1

CRN 189367-54-2

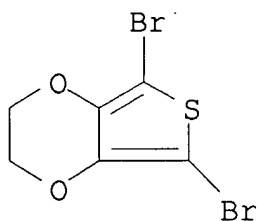
CMF C25 H32 Br2



CM 2

CRN 174508-31-7

CMF C6 H4 Br2 O2 S



- IT Polymers, preparation
(conjugated; improved hole-injecting properties of copolymers dihexylfluorene with ethylenedioxythiophene)
- IT Cyclic voltammetry
Electric current
Electroluminescent devices
Light
Luminescence
Luminescence, electroluminescence
Molecular weight distribution
Optical absorption
UV radiation
(improved hole-injecting properties of copolymers dihexylfluorene with ethylenedioxythiophene)
- IT Thickness
(thickness effect of conducting polymer on electroluminescent device)
- IT 7440-66-6, Zinc, uses
(activated, polymn. catalyst; improved hole-injecting properties

- of copolymers dihexylfluorene with ethylenedioxythiophene)
- IT 163359-60-2 350037-71-7, 2,5-Dibromo-3,4-ethylenedioxythiophene homopolymer
(improved hole-injecting properties of copolymers dihexylfluorene with ethylenedioxythiophene)
- IT 498358-35-3P
(improved hole-injecting properties of copolymers dihexylfluorene with ethylenedioxythiophene)
- IT 133019-09-7P, Poly(9,9-dihexyl-9H-fluorene-2,7-diyl) 201807-75-2P, 2,7-Dibromo-9,9-dihexylfluorene homopolymer
(improved hole-injecting properties of copolymers dihexylfluorene with ethylenedioxythiophene)
- IT 111-25-1, 1-Bromohexane 16433-88-8, 2,7-Dibromofluorene
(monomer synthesis; improved hole-injecting properties of copolymers dihexylfluorene with ethylenedioxythiophene)
- IT 189367-54-2P, 2,7-Dibromo-9,9-di-n-hexyl-fluorene
(monomer; improved hole-injecting properties of copolymers dihexylfluorene with ethylenedioxythiophene)
- IT 603-35-0, Triphenylphosphine, uses 46389-47-3, 2,2'-Bipyridine Nickel dibromide
(polymn. catalyst; improved hole-injecting properties of copolymers dihexylfluorene with ethylenedioxythiophene)

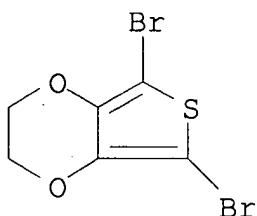
L26 ANSWER 15 OF 29 HCA COPYRIGHT 2005 ACS on STN

137:85573 Dihexyl-fluorene-co-3,4 ethylenedioxythiophene copolymers for OLEDs. Stephan, Olivier; Tran-Van, Francois; Contat, Jerome; Dubois, Angelique; Chevrot, Claude (Laboratoire de Spectrometrie Physique, Universite Joseph Fourier Grenoble 1, Saint Martin d'Heres, 38402, Fr.). Materials Research Society Symposium Proceedings, 660(Organic Electronic and Photonic Materials and Devices), JJ1.5/1-JJ1.5/6 (English) 2001. CODEN: MRSPDH. ISSN: 0272-9172. Publisher: Materials Research Society.

AB The authors report synthesis, and optical properties, of dihexyl-fluorene-co-3,4-ethylenedioxythiophene (DHF-co-EDOT) random copolymers obtained from mixt., in various ratios, of the two corresponding dibrominated monomers. IR studies coupled with ¹H NMR clearly indicate, as expected, that the amt. of each monomer unit in the materials is strongly connected to the feed compn. It clearly appears that even a low 3,4-ethylenedioxythiophene (EDOT) content, i.e. 15%, within a poly(dihexyl fluorene) main chain induces significant changes in the electronic properties of the corresponding material, denoted COP01, compared with the fluorene-based homopolymer. Higher EDOT contents lead to less sol. copolymers which are not or only to a slight extent suitable to study their use as luminescent semiconducting π -conjugated materials in Org. Light-Emitting Diodes (OLEDs). Green org. light emitting devices based on COP01, exhibiting no significant spectral evolution, were demonstrated and showed improved hole-injection

properties when compared to the ones using poly(dihexyl fluorene). The use of an addnl. PEDOT-PSS layer on the ITO anode also was studied leading to improved operating lifetime.

IT 350037-71-7P
(dihexyl-fluorene-co-3,4 ethylenedioxythiophene copolymers for OLEDs)
RN 350037-71-7 HCA
CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro-, homopolymer (9CI) (CA INDEX NAME)
CM 1
CRN 174508-31-7
CMF C6 H4 Br2 O2 S



IT Electroluminescent devices
(org.; dihexyl-fluorene-co-3,4 ethylenedioxythiophene copolymers for OLEDs)
IT NMR (nuclear magnetic resonance)
(proton; dihexyl-fluorene-co-3,4 ethylenedioxythiophene copolymers for OLEDs)
IT 7429-90-5, Aluminum, uses 50926-11-9, Indium tin oxide
(dihexyl-fluorene-co-3,4 ethylenedioxythiophene copolymers for OLEDs)
IT 126213-51-2P, PEDOT 138184-36-8P 201807-75-2P
350037-71-7P 403986-27-6P
(dihexyl-fluorene-co-3,4 ethylenedioxythiophene copolymers for OLEDs)
IT 50851-57-5 123863-98-9, Poly(9,9-dihexylfluorene)
(dihexyl-fluorene-co-3,4 ethylenedioxythiophene copolymers for OLEDs)

L26 ANSWER 16 OF 29 HCA COPYRIGHT 2005 ACS on STN
137:20713 Vinylene-linked donor-acceptor polymers. Madrigal, Luis G.; Pinto, Mauricio; Schanze, Kirk S.; Reynolds, John R. (Dep. Chem., Center Macromolecular Sci. Eng., Univ. Florida, Gainesville, FL, 32611, USA). Polymer Preprints (American Chemical Society, Division of Polymer Chemistry), 43(1), 565 (English) 2002. CODEN: ACPPAY. ISSN: 0032-3934. Publisher: American Chemical Society, Division of

Polymer Chemistry.

AB Vinylene-linked donor-acceptor polymers were synthesized to obtain materials with low electronic band gap and accessible oxidative and reductive states. The Heck reaction was used to prep. poly(2,5-pyridyl vinylene-1,4-hexadecyloxy-phenylene vinylene) (P1), poly(2,3-diphenyl[3,4-b]-pyridopyrazine vinylene-1,4-hexadecyloxy phenylene vinylene) (P2), and poly(propylenedioxythiophene-MeOC16H33 vinylene-1,4-pyridyl vinylene) (P3). The polyphenylenevinylenes exhibit optical band gap of 2.4, 2.0, and 2.4 eV resp. The mol. wt. of these sol. polymers is 8,700 to 33,000 g/mol as detd. by GPC vs. polystyrene std. Doping of the polymers with antimony pentachloride led to formation of new red-shifted optical absorption bands characteristic of charge transfer species. A small pos. solvatochromism was obsd. from fluorescence spectra in solvents with distinct polarity but nearly the same Hildebrand soly. parameter; a relatively large Stokes-shift was also obsd.

IT 434935-11-2P

(prepn. and optical band gap and solvatochromism of fluorescent vinylene-linked pyridyl- and pyridopyrazine- and propylenedioxythiophene-contg. donor-acceptor conjugated polymers)

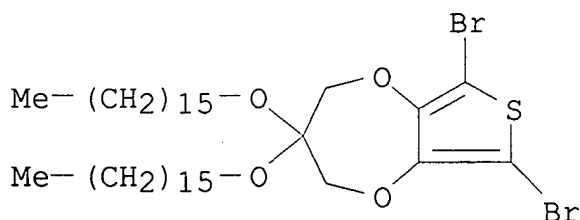
RN 434935-11-2 HCA

CN Pyridine, 2,5-diethenyl-, polymer with 6,8-dibromo-3,3-bis(hexadecyloxy)-3,4-dihydro-2H-thieno[3,4-b][1,4]dioxepin (9CI)
(CA INDEX NAME)

CM 1

CRN 434935-10-1

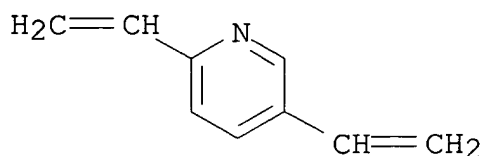
CMF C39 H70 Br2 O4 S



CM 2

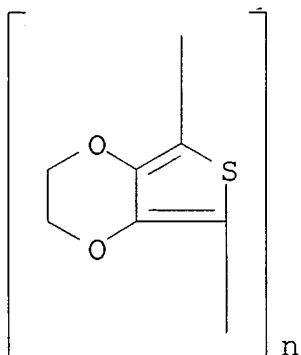
CRN 16222-95-0

CMF C9 H9 N



- IT Polymers, preparation
(conjugated; prepn. and optical band gap and solvatochromism of fluorescent vinylene-linked pyridyl- and pyridopyrazine- and propylenedioxythiophene-contg. donor-acceptor conjugated polymers)
- IT Band gap
(optical; prepn. and optical band gap and solvatochromism of fluorescent vinylene-linked pyridyl- and pyridopyrazine- and propylenedioxythiophene-contg. donor-acceptor conjugated polymers)
- IT Conducting polymers
(polythiophenes, pyridyl-contg.; prepn. and optical band gap and solvatochromism of fluorescent vinylene-linked pyridyl- and pyridopyrazine- and propylenedioxythiophene-contg. donor-acceptor conjugated polymers)
- IT Charge transfer interaction
Excited state absorption
Optical absorption edge
Polarized fluorescence
Solvatochromism
(prepn. and optical band gap and solvatochromism of fluorescent vinylene-linked pyridyl- and pyridopyrazine- and propylenedioxythiophene-contg. donor-acceptor conjugated polymers)
- IT Poly(arylenealkenylenes)
(pyridyl and pyridopyrazine contg.; prepn. and optical band gap and solvatochromism of fluorescent vinylene-linked pyridyl- and pyridopyrazine- and propylenedioxythiophene-contg. donor-acceptor conjugated polymers)
- IT 7647-18-9, Antimony pentachloride
(dopant; prepn. and optical band gap and solvatochromism of fluorescent vinylene-linked pyridyl- and pyridopyrazine- and propylenedioxythiophene-contg. donor-acceptor conjugated polymers)
- IT 178667-14-6P 178900-73-7P 434935-09-8P 434935-11-2P
434943-09-6P 434943-10-9P
(prepn. and optical band gap and solvatochromism of fluorescent vinylene-linked pyridyl- and pyridopyrazine- and propylenedioxythiophene-contg. donor-acceptor conjugated polymers)

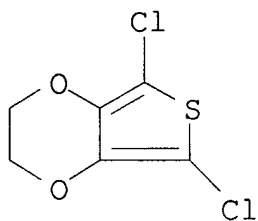
- IT 108-94-1, Cyclohexanone, uses
(solvent; prepn. and optical band gap and solvatochromism of
fluorescent vinylene-linked pyridyl- and pyridopyrazine- and
propylenedioxythiophene-contg. donor-acceptor conjugated
polymers)
- L26 ANSWER 17 OF 29 HCA COPYRIGHT 2005 ACS on STN
136:200547 Neutral poly(3,4-ethylenedioxythiophene-2,5-diyl)s:
preparation by organometallic polycondensation and their unique
p-doping behavior. Yamamoto, Takakazu; Shiraishi, Kouichi; Abla,
Mahmut; Yamaguchi, Isao; Groenendaal, L. "Bert" (Chemical Resources
Laboratory, Tokyo Institute of Technology, Yokohama, Midori-ku,
226-8503, Japan). Polymer, Volume Date 2002, 43(3), 711-719
(English) 2001. CODEN: POLMAG. ISSN: 0032-3861. Publisher:
Elsevier Science Ltd..
- AB Neutral and non-doped poly(3,4-ethylenedioxythiophene), PEDOT_h(Ni),
and its hexyl deriv., PEDOT_h-C₆(Ni), have been prepd. by
organometallic dehalogenation polycondensation of
2,5-dichloro-3,4-ethylenedioxythiophene and its hexyl deriv. with a
zerovalent nickel complex. PEDOT_h-C₆(Ni) was sol. in org. solvents
and ¹H NMR data indicated that it had an Mn of 11,000. MALDI-TOF
mass anal. of PEDOT_h(Ni) gave Mn and Mw of about 1700 and 2400,
resp. PEDOT_h-C₆(Ni) showed a UV-Vis absorption peak at 546 nm in
CHCl₃. Electrochem. oxidn. of PEDOT_h-C₆(Ni) started at about -0.40
V vs Ag⁺/Ag and gave a peak at 0.20 V vs Ag⁺/Ag. Chem. and
electrochem. oxidn. (or p-doping) of PEDOT_h-C₆(Ni), both in solns.
and in a solid state, led to weakening of the original π - π^*
peaks and rise of new peak(s) in a region of 800-1500 nm. The
p-doping of PEDOT_h-C₆(Ni) caused not only a decrease in the
intensity of ¹H NMR signals of the bridging ethylene hydrogens but
also a decrease in that of the hexyl side chain, suggesting a strong
interaction of the p-dopant with the side chain. NMR data of
poly(3-methoxythiophene-2,5-diyl) also supported an assumption that
p-doping brings about a severe change in electronic state of the
substituent attached to the polythiophene main chain. PEDOT_h(Ni)
had a d. of 1.71 g cm⁻³; the mol. packing mode of PEDOT_h(Ni) is
discussed based on the d. of the polymer and its XRD data.
- IT 163359-60-2P 225518-50-3P 350827-43-9P
(prepn. of neutral poly(ethylenedioxythiophenediyl)s by
organometallic polycondensation and their unique p-doping
behavior)
- RN 163359-60-2 HCA
CN Poly(2,3-dihydrothieno[3,4-b]-1,4-dioxin-5,7-diyl) (9CI) (CA INDEX
NAME)



RN 225518-50-3 HCA
 CN Thieno[3,4-b]-1,4-dioxin, 5,7-dichloro-2,3-dihydro-, homopolymer
 (9CI) (CA INDEX NAME)

CM 1

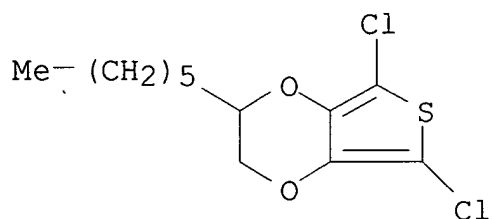
CRN 225518-49-0
 CMF C6 H4 Cl2 O2 S



RN 350827-43-9 HCA
 CN Thieno[3,4-b]-1,4-dioxin, 5,7-dichloro-2-hexyl-2,3-dihydro-,
 homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 350827-42-8
 CMF Cl2 H16 Cl2 O2 S

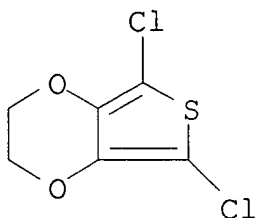


IT 225518-49-0P 350827-42-8P

(prepn. of neutral poly(ethylenedioxythiophenediyl)s by organometallic polycondensation and their unique p-doping behavior)

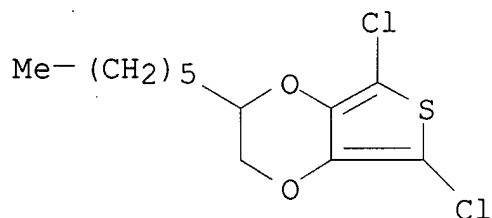
RN 225518-49-0 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dichloro-2,3-dihydro- (9CI) (CA INDEX NAME)



RN 350827-42-8 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dichloro-2-hexyl-2,3-dihydro- (9CI) (CA INDEX NAME)



IT Electric conductivity

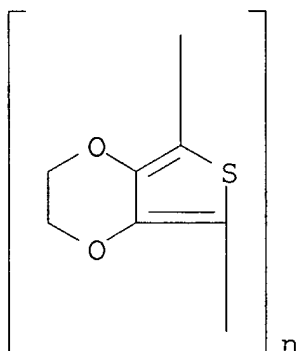
(prepn. of neutral poly(ethylenedioxythiophenediyl)s by organometallic polycondensation and their unique p-doping behavior)

IT 163359-60-2P 225518-50-3P 350827-43-9P
351317-30-1P

(prepn. of neutral poly(ethylenedioxythiophenediyl)s by organometallic polycondensation and their unique p-doping behavior)

- behavior)
- IT 126213-50-1 126213-53-4
(prepn. of neutral poly(ethylenedioxythiophenediyl)s by organometallic polycondensation and their unique p-doping behavior)
- IT 225518-49-0P 350827-42-8P
(prepn. of neutral poly(ethylenedioxythiophenediyl)s by organometallic polycondensation and their unique p-doping behavior)
- L26 ANSWER 18 OF 29 HCA COPYRIGHT 2005 ACS on STN
- 135:242592 Optical and electrochemical properties of soluble N-hexylcarbazole-co-3,4-ethylenedioxythiophene copolymers. Beouch, L.; Tran Van, F.; Stephan, O.; Vial, J. C.; Chevrot, C. (Equipe Reactivite aux Interfaces (EA 2528), Laboratoire sur les Polymeres et les Materiaux Electroactifs, Universite de Cergy Pontoise, Cergy Pontoise, 95013, Fr.). Synthetic Metals, 122(2), 351-358 (English) 2001. CODEN: SYMEDZ. ISSN: 0379-6779. Publisher: Elsevier Science S.A..
- AB Sol. N-hexylcarbazole-co-3,4-ethylenedioxythiophene (HCz-co-EDOT) copolymers from mixts. in various ratio of the two corresponding dihalogenated monomers were synthesized. The random copolymers were obtained from EDOT/HCz starting molar ratio: 0.25, 1, 4, named, resp., C1, C2 and C3, and compared their properties to the two homopolymers synthesized in the same way. The IR studies clearly indicated, that an increase in the amt. of ethylenedioxythiophene in the feed compn. leads to an increase of the proportion of the corresponding comonomer in the final materials. Elemental anal. point out that the reactivity of dibrominated EDOT seems slightly lower than that of dibrominated HCz. Thin films of copolymer have been prepd. and their electrochem. response have been investigated. Absorption and luminescence of these materials have been also studied in CHCl3. Copolymers mainly composed of one monomer (C1 and C3) behaves like the corresponding homopolymers. On an other hand, copolymer (C2) obtained from an equimolar amt. of each monomer in the feed compn. clearly exhibits distinct signals in optical spectra and in electrochem. behavior, probably due to the presence of each monomer unit short segments. The use of C2 has been explored for possible application in light emitting devices indicating that the p-doping of the material would be facilitated leading to an improved hole injecting when compared to carbazole homopolymer. It could be particularly interesting as a hole transporting layer in multilayer org. light emitting devices.
- IT 163359-60-2P 350037-71-7P 359829-16-6P
(optical and electrochem. properties of sol. N-hexylcarbazole-co-3,4-ethylenedioxythiophene copolymers)
- RN 163359-60-2 HCA
- CN Poly(2,3-dihydrothieno[3,4-b]-1,4-dioxin-5,7-diyl) (9CI) (CA INDEX

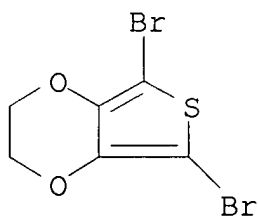
NAME)



RN 350037-71-7 HCA
 CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro-, homopolymer
 (9CI) (CA INDEX NAME)

CM 1

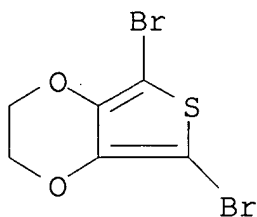
CRN 174508-31-7
 CMF C6 H4 Br2 O2 S



RN 359829-16-6 HCA
 CN 9H-Carbazole, 3,6-dibromo-9-hexyl-, polymer with
 5,7-dibromo-2,3-dihydrothieno[3,4-b]-1,4-dioxin (9CI) (CA INDEX
 NAME)

CM 1

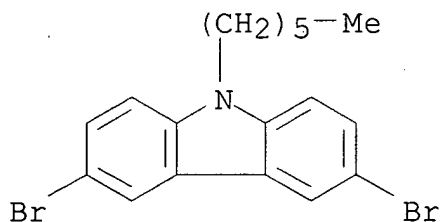
CRN 174508-31-7
 CMF C6 H4 Br2 O2 S



CM 2

CRN 150623-72-6

CMF C18 H19 Br2 N

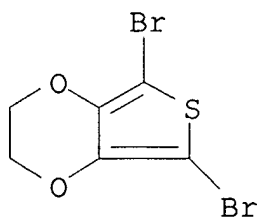


IT 174508-31-7P

(optical and electrochem. properties of sol. N-hexylcarbazole-co-3,4-ethylenedioxythiophene copolymers)

RN 174508-31-7 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro- (9CI) (CA INDEX NAME)



IT Absorption spectra

Cyclic voltammetry

Fluorescence

Hole transport

Luminescence

Luminescence, electroluminescence

(optical and electrochem. properties of sol. N-hexylcarbazole-co-

- 3,4-ethylenedioxythiophene copolymers)
- IT Band gap
(optical; optical and electrochem. properties of sol.
N-hexylcarbazole-co-3,4-ethylenedioxythiophene copolymers)
- IT Polymers, preparation
(polythiophenes, carbazole group-contg.; optical and electrochem.
properties of sol. N-hexylcarbazole-co-3,4-ethylenedioxythiophene
copolymers)
- IT 7440-66-6, Zinc, uses
(activated; optical and electrochem. properties of sol.
N-hexylcarbazole-co-3,4-ethylenedioxythiophene copolymers)
- IT 56-37-1, Triethylbenzylammonium chloride
(optical and electrochem. properties of sol. N-hexylcarbazole-co-
3,4-ethylenedioxythiophene copolymers)
- IT **163359-60-2P 350037-71-7P 359829-15-5P**
359829-16-6P 359829-17-7P, Poly(9-hexyl-9H-carbazole-3,6-
diyl)
(optical and electrochem. properties of sol. N-hexylcarbazole-co-
3,4-ethylenedioxythiophene copolymers)
- IT 111-25-1, Hexyl bromide 128-08-5, N-Bromosuccinimide 6825-20-3,
3,6-Dibromocarbazole 126213-50-1, 3,4-Ethylenedioxythiophene
(optical and electrochem. properties of sol. N-hexylcarbazole-co-
3,4-ethylenedioxythiophene copolymers)
- IT 150623-72-6P **174508-31-7P**
(optical and electrochem. properties of sol. N-hexylcarbazole-co-
3,4-ethylenedioxythiophene copolymers)
- IT 46389-47-3, 2,2'-Bipyridinenickel dibromide
(polymn. catalyst; optical and electrochem. properties of sol.
N-hexylcarbazole-co-3,4-ethylenedioxythiophene copolymers)

L26 ANSWER 19 OF 29 HCA COPYRIGHT 2005 ACS on STN

135:122840 Preparation of a soluble and neutral alkyl derivative of
poly(3,4-ethylene-dioxythiophene) and its optical properties.
Shiraishi, K.; Kanbara, T.; Yamamoto, T.; Groenendaal, L. B.
(Chemical Resources Laboratory, Tokyo Institute of Technology,
Nagatsuta, Midori-ku, Yokohama, 226-8503, Japan). Polymer, 42(16),
7229-7232 (English) 2001. CODEN: POLMAG. ISSN: 0032-3861.
Publisher: Elsevier Science Ltd..

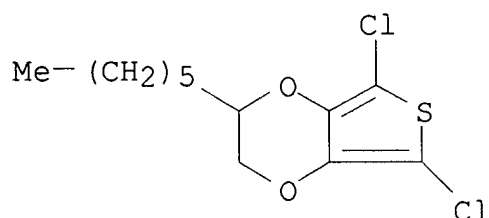
AB Sol. and non-doped poly(3,4-ethylenedioxythiophene) with a hexyl
substituent (PEDOTh-C6 (Ni)), was first synthesized by Ni promoted
dehalogenation polycondensation of the corresponding monomer.
PEDOTh-C6 (Ni) exhibited good soly. in common org. solvents such as
CHCl₃, CH₂Cl₂, and DMF, in contrast to poor soly. of the
corresponding polymer synthesized by oxidative polymn. GPC anal.
indicated that PEDOTh-C6 (Ni) had Mn and Mw of 5400 and 8500 (vs
polystyrene stds.); ¹H NMR anal. gave an Mn value of 11,000. A cast
film of PEDOTh-C6 (Ni) received electrochem. p-doping at 0.20 V vs
Ag⁺/Ag. Chem. and electrochem. oxidn. of PEDOTh-C6 (Ni) led to

appearance of new absorption bands in the near IR region.

IT **350827-43-9P**
 (prepn. of a sol. and neutral hexyl deriv. of
 poly(3,4-ethylene-dioxythiophene) and optical properties of
 nondoped and doped polymers)
 RN 350827-43-9 HCA
 CN Thieno[3,4-b]-1,4-dioxin, 5,7-dichloro-2-hexyl-2,3-dihydro-,
 homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 350827-42-8
 CMF C12 H16 Cl2 O2 S



IT Dopants
 Doping
 UV and visible spectra
 (prepn. of a sol. and neutral hexyl deriv. of
 poly(3,4-ethylene-dioxythiophene) and optical properties of
 nondoped and doped polymers)
 IT 7553-56-2, Iodine, uses
 (dopant; prepn. of a sol. and neutral hexyl deriv. of
 poly(3,4-ethylene-dioxythiophene) and optical properties of
 nondoped and doped polymers)
 IT 350827-42-8P
 (monomer; prepn. of a sol. and neutral hexyl deriv. of
 poly(3,4-ethylene-dioxythiophene) and optical properties of
 nondoped and doped polymers)
 IT 1295-35-8, Bis(1,5-cyclooctadiene)nickel
 (polymn. catalyst; prepn. of a sol. and neutral hexyl deriv. of
 poly(3,4-ethylene-dioxythiophene) and optical properties of
 nondoped and doped polymers)
 IT **350827-43-9P** 351317-30-1P
 (prepn. of a sol. and neutral hexyl deriv. of
 poly(3,4-ethylene-dioxythiophene) and optical properties of
 nondoped and doped polymers)
 IT 128-09-6, N-Chlorosuccinimide
 (reactant in monomer prepn.; prepn. of a sol. and neutral hexyl
 deriv. of poly(3,4-ethylene-dioxythiophene) and optical

properties of nondoped and doped polymers)

L26 ANSWER 20 OF 29 HCA COPYRIGHT 2005 ACS on STN

135:108027 A fully undoped oligo(3,4-ethylenedioxythiophene): spectroscopic properties. Tran-Van, F.; Garreau, S.; Louarn, G.; Froyer, G.; Chevrot, C. (Laboratoire sur les Polymeres et les Materiaux Electroactifs, 5 mail Gay Lussac, Universite de Cergy Pontoise, Cergy Pontoise, 95013, Fr.). Synthetic Metals, 119(1-3), 381-382 (English) 2001. CODEN: SYMEDZ. ISSN: 0379-6779. Publisher: Elsevier Science S.A..

AB We present here the synthesis of fully undoped oligo(3,4-ethylenedioxythiophene) by a dehalogenation polycondensation route. Since it is partly sol., spectroscopic expts. like optical absorption were carried out. The oligomer was studied by means of Raman scattering, IR absorption and x-ray diffraction, and compared to the PEDOT obtained by oxidative way.

IT 350037-71-7DP, debrominated
(prepn. and spectroscopic characterization of)

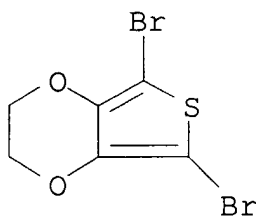
RN 350037-71-7 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro-, homopolymer
(9CI) (CA INDEX NAME)

CM 1

CRN 174508-31-7

CMF C6 H4 Br2 O2 S



IT 350037-71-7DP, debrominated
(prepn. and spectroscopic characterization of)

L26 ANSWER 21 OF 29 HCA COPYRIGHT 2005 ACS on STN

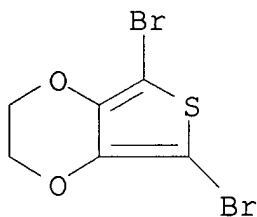
135:107664 Fully undoped and soluble oligo(3,4-ethylenedioxythiophene)s: spectroscopic study and electrochemical characterization. Tran-Van, Francois; Garreau, Sebastien; Louarn, Guy; Froyer, Gerard; Chevrot, Claude (Equipe Reactivite aux Interfaces (EA 2528), Laboratoire sur les Polymeres et les Materiaux Electroactifs, Universite de Cergy Pontoise, Cergy Pontoise, 95013, Fr.). Journal of Materials Chemistry, 11(5), 1378-1382 (English) 2001. CODEN: JMACEP. ISSN: 0959-9428. Publisher: Royal Society of Chemistry.

AB Fully undoped oligo(3,4-ethylenedioxythiophene)s were synthesized via polycondensation of the dibromo monomer in the presence of $\text{NiBr}_2(\text{bpy})$ catalyst in N,N -dimethylacetamide (DMA). HPLC anal. indicated that the material is constituted of three main oligomers which were clearly detected by UV-Visible spectroscopy. The polythiophenes are partially sol. in DMA making them easier to process to produce thin films of oligomers by evapn. of the solvent. Electrochem. and electrochromic properties of undoped films were studied. Deep purple in its undoped state, the material becomes sky blue in the oxidized form. The mixt. of oligomers was characterized by Raman scattering, IR absorption and X-Ray diffraction, and compared to poly(3,4-ethylenedioxy thiophene) obtained by the oxidative route.

IT **174508-31-7P**, 2,5-Dibromo-3,4-ethylenedioxythiophene
(monomer; prepn. and redox electrochem. of electroactive fully undoped and sol. oligo(3,4-ethylenedioxythiophene)s)

RN 174508-31-7 HCA

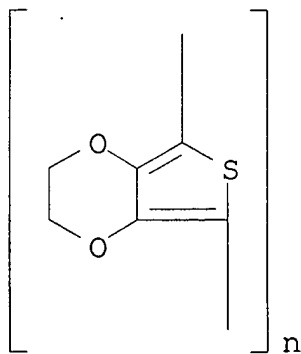
CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro- (9CI) (CA INDEX NAME)



IT **163359-60-2P 350037-71-7P**
(oligomeric; prepn. and redox electrochem. of electroactive fully undoped and sol. oligo(3,4-ethylenedioxythiophene)s)

RN 163359-60-2 HCA

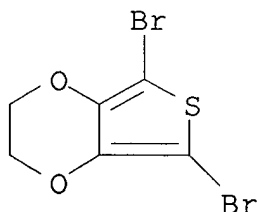
CN Poly(2,3-dihydrothieno[3,4-b]-1,4-dioxin-5,7-diyl) (9CI) (CA INDEX NAME)



RN 350037-71-7 HCA
 CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro-, homopolymer
 (9CI) (CA INDEX NAME)

CM 1

CRN 174508-31-7
 CMF C6 H4 Br2 O2 S



IT Polymers, preparation
 (conjugated; prepn. and redox electrochem. of electroactive fully undoped and sol. oligo(3,4-ethylenedioxythiophene)s)

IT Polymerization
 (dehalogenation condensation; prepn. and redox electrochem. of electroactive fully undoped and sol. oligo(3,4-ethylenedioxythiophene)s)

IT Redox reaction
 (electrochem.; prepn. and redox electrochem. of electroactive fully undoped and sol. oligo(3,4-ethylenedioxythiophene)s)

IT Polymer chains
 (length, conjugation, low homogeneity; prepn. and redox electrochem. of electroactive fully undoped and sol. oligo(3,4-ethylenedioxythiophene)s)

IT Polymers, preparation
 (polythiophenes, ethylenedioxythiophene, oligomeric; prepn. and redox electrochem. of electroactive fully undoped and sol. oligo(3,4-ethylenedioxythiophene)s)

IT Conducting polymers
 (polythiophenes; prepn. and redox electrochem. of electroactive fully undoped and sol. oligo(3,4-ethylenedioxythiophene)s)

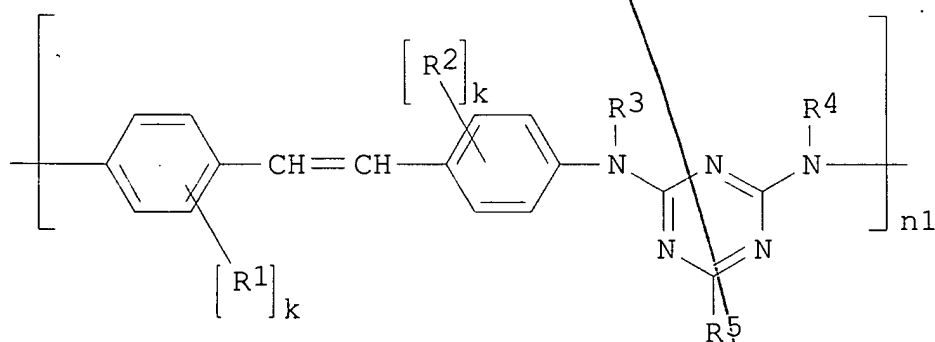
IT Conjugation (bond)
 Electrochromic materials
 Electrochromism
 Raman spectra
 Redox potential
 (prepn. and redox electrochem. of electroactive fully undoped and sol. oligo(3,4-ethylenedioxythiophene)s)

IT Band gap

- (semiconductor; prepn. and redox electrochem. of electroactive fully undoped and sol. oligo(3,4-ethylenedioxythiophene)s)
- IT 182628-58-6, (2,2'-Bipyridine)dibromonickel
(condensation polymn. catalyst; prepn. and redox electrochem. of electroactive fully undoped and sol. oligo(3,4-ethylenedioxythiophene)s)
- IT 174508-31-7P, 2,5-Dibromo-3,4-ethylenedioxythiophene
(monomer; prepn. and redox electrochem. of electroactive fully undoped and sol. oligo(3,4-ethylenedioxythiophene)s)
- IT 163359-60-2P 350037-71-7P
(oligomeric; prepn. and redox electrochem. of electroactive fully undoped and sol. oligo(3,4-ethylenedioxythiophene)s)
- IT 128-08-5, N-Bromosuccinimide 126213-50-1, 3,4-Ethylenedioxythiophene
(prepn. and redox electrochem. of electroactive fully undoped and sol. oligo(3,4-ethylenedioxythiophene)s)
- IT 127-19-5, N,N-Dimethylacetamide
(solvent; prepn. and redox electrochem. of electroactive fully undoped and sol. oligo(3,4-ethylenedioxythiophene)s)

L26 ANSWER 22 OF 29 HCA COPYRIGHT 2005 ACS on STN
135:68356 Organic electroluminescent device. Nakamura, Kazuaki; Ueda, Noriko; Yamada, Taketoshi; Kita, Hiroshi (Konica Co., Japan). Jpn. Kokai Tokkyo Koho JP 2001167885 A2 20010622, 44 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 2000-286785 20000921. PRIORITY: JP 1999-276616 19990929.

GI



AB The invention relates to an org. electroluminescent device that emits in UV-violet region, comprising a polymer represented by I [R1-R4 = substitution groups; R5 = H or substitution group; k and m = 0-4 integer; when k and m ≥ 2 , condensed ring may be formed]

among R1 and R2; n1 = 1-5,000 integer].

IT 345665-81-8 345666-05-9 345666-11-7

(org. electroluminescent device)

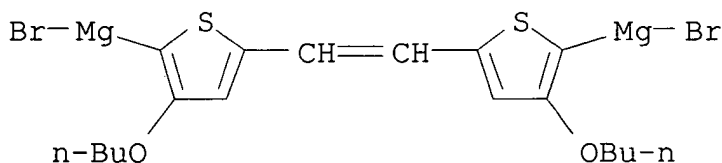
RN 345665-81-8 HCA

CN Magnesium, dibromo[μ -[1,2-ethenediylbis(3-butoxy-5,2-thiophenediyl)]]di-, polymer with 2,5-dibromo-3,4-dibutoxythiophene (9CI) (CA INDEX NAME)

CM 1

CRN 345665-80-7

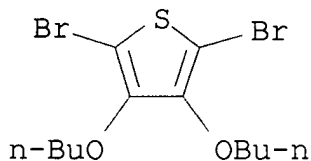
CMF C18 H22 Br2 Mg2 O2 S2



CM 2

CRN 173291-49-1

CMF C12 H18 Br2 O2 S



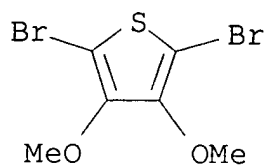
RN 345666-05-9 HCA

CN Magnesium, dibromo[μ -[1,2-ethenediylbis(3-methyl-5,2-thiophenediyl)]]di-, polymer with 2,5-dibromo-3,4-dimethoxythiophene (9CI) (CA INDEX NAME)

CM 1

CRN 345666-04-8

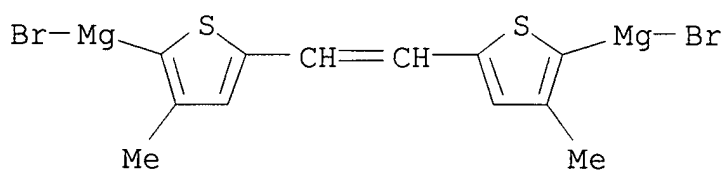
CMF C6 H6 Br2 O2 S



CM 2

CRN 345666-03-7

CMF C12 H10 Br2 Mg2 S2



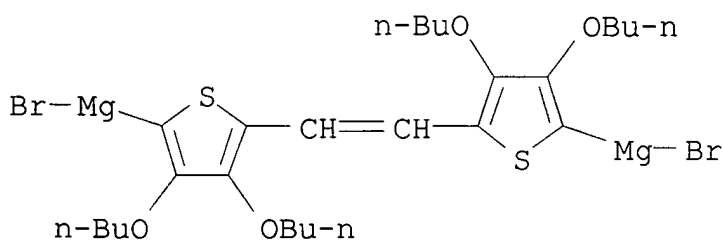
RN 345666-11-7 HCA

CN Magnesium, dibromo[μ-[1,2-ethenediylbis(3,4-dibutoxy-5,2-thiophenediyl)]]di-, polymer with 2,5-dibromo-3,4-dimethoxythiophene (9CI) (CA INDEX NAME)

CM 1

CRN 345666-10-6

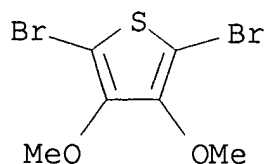
CMF C26 H38 Br2 Mg2 O4 S2



CM 2

CRN 345666-04-8

CMF C6 H6 Br2 O2 S

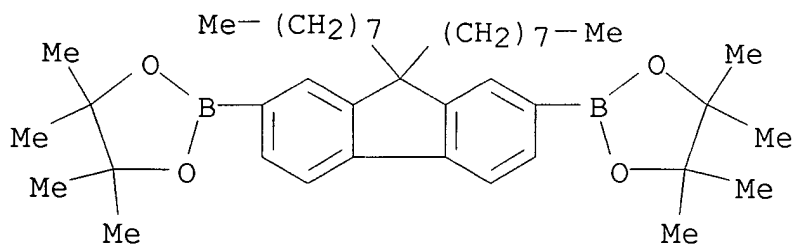


- IT Optical filters
(color conversion; org. electroluminescent device)
- IT Electroluminescent devices
(org. electroluminescent device)
- IT Polyamides, uses
(org. electroluminescent device)
- IT 345665-75-0 345665-76-1 345665-77-2 345665-79-4
345665-81-8 345665-82-9 345665-84-1 345665-85-2
 345665-86-3 345665-87-4 345665-88-5 345665-90-9 345665-92-1
 345665-94-3 345665-96-5 345665-98-7 345666-00-4 345666-02-6
345666-05-9 345666-07-1 345666-09-3 **345666-11-7**
 (org. electroluminescent device)
- L26 ANSWER 23 OF 29 HCA COPYRIGHT 2005 ACS on STN
- 133:208463 Molecular Design and Characterization of Chromic Polyfluorene Derivatives. Blondin, Pierre; Bouchard, Jimmy; Beaupre, Serge; Belletete, Michel; Durocher, Gilles; Leclerc, Mario (Departement de Chimie Centre de Recherche en Sciences et Ingenierie des Macromolecules, Universite Laval, Quebec, QC, G1K 7P4, Can.). Macromolecules, 33(16), 5874-5879 (English) 2000. CODEN: MAMOBX. ISSN: 0024-9297. Publisher: American Chemical Society.
- AB The thermochromic and solvatochromic properties of a series of fluorene-based conjugated polymers have been investigated. Both poly(2,7-(9,9-dioctylfluorene)) and poly(2,5-(thiophene)-alt-2,7-(9,9-dioctylfluorene)) have revealed interesting chromic properties which, on the basis of theor. calcns., seem to be related to a relatively flexible backbone. On the other hand, the sterically hindered, nonplanar poly(2,5-(3,4-dimethylthiophene)-alt-2,7-(9,9-dioctylfluorene)) does not exhibit any significant solvatochromic and thermochromic properties which could be explained by an important energy barrier against planarity. Finally, investigations on poly(2,5-(3,4-ethylenedioxythiophene)-alt-2,7-(9,9-dioctylfluorene)) have revealed a highly conjugated conformational structure which is not significantly modified upon temp. or solvent changes.
- IT **287924-59-8 287924-60-1**
(mol. design and characterization of chromic polyfluorene derivs.)
- RN 287924-59-8 HCA
- CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro-, polymer with

2,2'-(9,9-dioctyl-9H-fluorene-2,7-diyl)bis[4,4,5,5-tetramethyl-1,3,2-dioxaborolane] (9CI) (CA INDEX NAME)

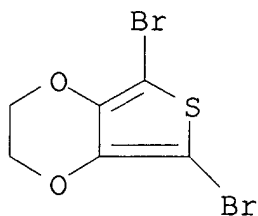
CM 1

CRN 196207-58-6
CMF C41 H64 B2 O4



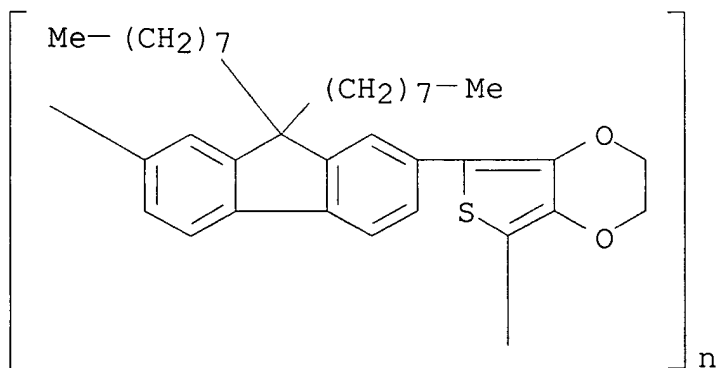
CM 2

CRN 174508-31-7
CMF C6 H4 Br2 O2 S

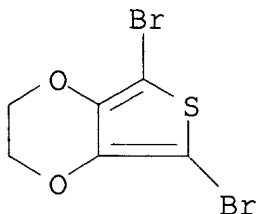


RN 287924-60-1 HCA

CN Poly[(2,3-dihydrothieno[3,4-b]-1,4-dioxin-5,7-diyl) (9,9-dioctyl-9H-fluorene-2,7-diyl)] (9CI) (CA INDEX NAME)



IT 174508-31-7P, 2,5-Dibromo-3,4-ethylenedioxythiophene
(mol. design and characterization of chromic polyfluorene
derivs.)
RN 174508-31-7 HCA
CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro- (9CI) (CA INDEX
NAME)



IT Polymers, properties
(fluorene-based; mol. design and characterization of chromic
polyfluorene derivs.)
IT Potential barrier
Potential energy
Solvatochromism
Thermochromism
UV and visible spectra
(mol. design and characterization of chromic polyfluorene
derivs.)
IT Bond angle
(torsional; mol. design and characterization of chromic
polyfluorene derivs.)
IT 123864-00-6, Poly(9,9-dioctylfluorene) 222857-60-5 222857-62-7
287924-57-6 287924-58-7 287924-59-8 287924-60-1
(mol. design and characterization of chromic polyfluorene
derivs.)
IT 3141-26-2, 3,4-Dibromothiophene
(mol. design and characterization of chromic polyfluorene
derivs.)
IT 74707-05-4P, 2,5-Dibromo-3,4-dimethylthiophene 174508-31-7P
, 2,5-Dibromo-3,4-ethylenedioxythiophene
(mol. design and characterization of chromic polyfluorene
derivs.)

L26 ANSWER 24 OF 29 HCA COPYRIGHT 2005 ACS on STN
133:164431 Light-Emitting Diodes from Fluorene-Based π -Conjugated
Polymers. Donat-Bouillud, Anne; Levesque, Isabelle; Tao, Ye;
D'Iorio, Marie; Beaupre, Serge; Blondin, Pierre; Ranger, Maxime;
Bouchard, Jimmy; Leclerc, Mario (Institute for Microstructural
Sciences, National Research Council of Canada, Ottawa, ON, K1A 0R6,

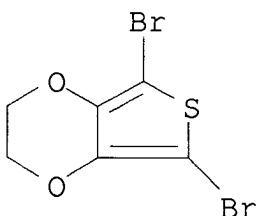
Can.). Chemistry of Materials, 12(7), 1931-1936 (English) 2000.
CODEN: CMATEX. ISSN: 0897-4756. Publisher: American Chemical
Society.

AB The synthesis of fluorene-based π -conjugated polymers was carried out and the electroluminescent properties of the polymers were studied. The photo- and electroluminescence of poly(dioctylfluorene-phenylene)s and poly(dioctylfluorene-thiophene)s whose synthesis was recently published was also studied. The alternate incorporation of phenylene or thiophene moieties in fluorene-based π -conjugated polymers was used to effect tunability of electroluminescent properties. The spectral emission varies from blue to green or yellow, depending on the compn. of the copolymers. To enhance the luminescence efficiency of polymer assemblies, hole injection and hole transport into the polymer were improved by insertion of an insulating buffer layer and the incorporation of efficient hole transport material in the polymer. The insertion of a charge injection layer such as LiF and a hole transport layer such as N,N'-diphenyl-N,N'-bis(3-methylphenyl)-1,1-biphenyl-4,4'-diamine significantly improved the electroluminescence efficiency of a test diode from 4.5 to 125 cd/m².

IT **174508-31-7P**, 2,5-Dibromo-3,4-ethylenedioxythiophene
(monomer; prepn. of poly(dioctylfluorene-thiophene)s with tunable electroluminescence and improved carrier transport for use in light-emitting diodes)

RN 174508-31-7 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro- (9CI) (CA INDEX NAME)



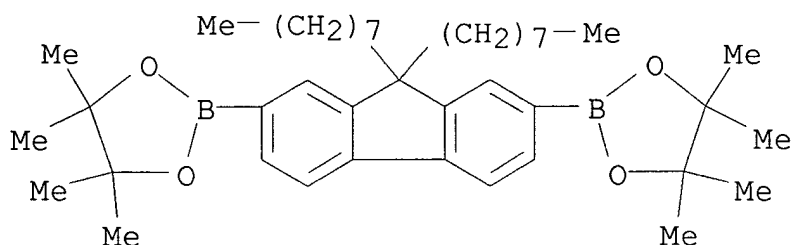
IT **287924-59-8P 287924-60-1P 287924-61-2P**
287924-62-3P

(prepn. of poly(dioctylfluorene-thiophene)s with tunable electroluminescence and improved carrier transport for use in light-emitting diodes)

RN 287924-59-8 HCA

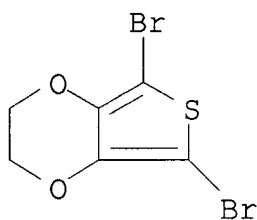
CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro-, polymer with 2,2'-(9,9-dioctyl-9H-fluorene-2,7-diyl)bis[4,4,5,5-tetramethyl-1,3,2-dioxaborolane] (9CI) (CA INDEX NAME)

CRN 196207-58-6
CMF C41 H64 B2 O4

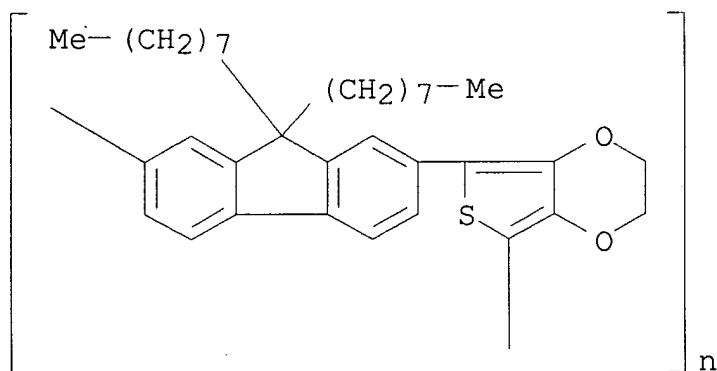


CM 2

CRN 174508-31-7
CMF C6 H4 Br2 O2 S



RN 287924-60-1 HCA
CN Poly[(2,3-dihydrothieno[3,4-b]-1,4-dioxin-5,7-diyl)(9,9-dioctyl-9H-fluorene-2,7-diyl)] (9CI) (CA INDEX NAME)



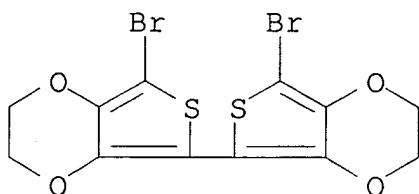
RN 287924-61-2 HCA
CN 5,5'-Bithieno[3,4-b]-1,4-dioxin, 7,7'-dibromo-2,2',3,3'-tetrahydro-, polymer with 2,2'-(9,9-dioctyl-9H-fluorene-2,7-diyl)bis[4,4,5,5-

tetramethyl-1,3,2-dioxaborolane] (9CI) (CA INDEX NAME)

CM 1

CRN 287924-56-5

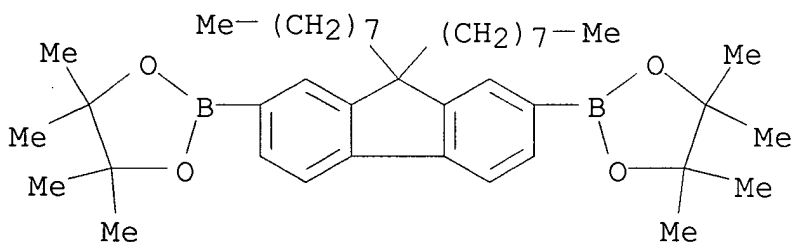
CMF C12 H8 Br2 O4 S2



CM 2

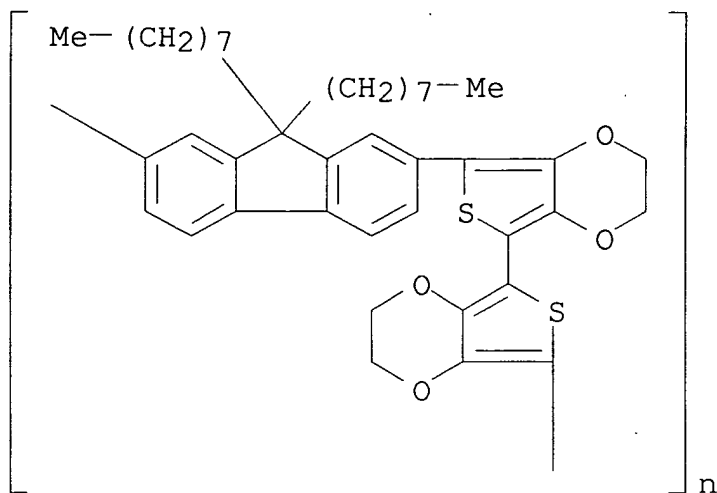
CRN 196207-58-6

CMF C41 H64 B2 O4



RN 287924-62-3 HCA

CN Poly[(2,2',3,3'-tetrahydro[5,5'-bithieno[3,4-b]-1,4-dioxin]-7,7'-diyl)(9,9-dioctyl-9H-fluorene-2,7-diyl)] (9CI) (CA INDEX NAME)

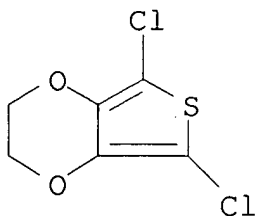


- IT Polymerization
(Suzuki coupling; prepn. of poly(dioctylfluorene-thiophene)s with tunable electroluminescence and improved carrier transport for use in light-emitting diodes)
- IT Polymers, preparation
(conjugated; prepn. of poly(dioctylfluorene-thiophene)s with tunable electroluminescence and improved carrier transport for use in light-emitting diodes)
- IT Electroluminescent devices
(light emitting diodes; prepn. of poly(dioctylfluorene-thiophene)s with tunable electroluminescence and improved carrier transport for use in light-emitting diodes)
- IT Polymers, preparation
(polythiophenes, polyfluorene; prepn. of poly(dioctylfluorene-thiophene)s with tunable electroluminescence and improved carrier transport for use in light-emitting diodes)
- IT Conducting polymers
Electrochromism
Hole transport
Luminescence, electroluminescence
Oxidation potential
Reduction potential
Suzuki coupling reaction
(prepn. of poly(dioctylfluorene-thiophene)s with tunable electroluminescence and improved carrier transport for use in light-emitting diodes)
- IT Electric current carriers
(transport; prepn. of poly(dioctylfluorene-thiophene)s with tunable electroluminescence and improved carrier transport for use in light-emitting diodes)

- IT 7789-24-4, Lithium fluoride (LiF), properties
(carrier injection layer; prepn. of poly(dioctylfluorene-thiophene)s with tunable electroluminescence and improved carrier transport for use in light-emitting diodes)
- IT 65181-78-4, N,N'-Diphenyl-N,N'-bis(3-methylphenyl)-1,1-biphenyl-4,4'-diamine
(hole transport layer; prepn. of poly(dioctylfluorene-thiophene)s with tunable electroluminescence and improved carrier transport for use in light-emitting diodes)
- IT 195602-17-6P, 2,2'-Bis(3,4-ethylenedioxy)bithiophene
(monomer and intermediate; prepn. of poly(dioctylfluorene-thiophene)s with tunable electroluminescence and improved carrier transport for use in light-emitting diodes)
- IT 74707-05-4P, 2,5-Dibromo-3,4-dimethylthiophene **174508-31-7P**
, 2,5-Dibromo-3,4-ethylenedioxythiophene 287924-56-5P
(monomer; prepn. of poly(dioctylfluorene-thiophene)s with tunable electroluminescence and improved carrier transport for use in light-emitting diodes)
- IT 7440-05-3, Palladium, uses
(polymn. catalyst; prepn. of poly(dioctylfluorene-thiophene)s with tunable electroluminescence and improved carrier transport for use in light-emitting diodes)
- IT 198964-57-7P 198964-62-4P 210347-56-1P 222857-60-5P
222857-62-7P 222857-64-9P 222857-68-3P 222857-69-4P
287924-57-6P 287924-58-7P **287924-59-8P**
287924-60-1P 287924-61-2P 287924-62-3P
(prepn. of poly(dioctylfluorene-thiophene)s with tunable electroluminescence and improved carrier transport for use in light-emitting diodes)
- IT 75-16-1, Methylmagnesium bromide 128-08-5, NBS 3141-26-2,
3,4-Dibromothiophene 126213-50-1, 3,4-Ethylenedioxythiophene
(prepn. of poly(dioctylfluorene-thiophene)s with tunable electroluminescence and improved carrier transport for use in light-emitting diodes)
- L26 ANSWER 25 OF 29 HCA COPYRIGHT 2005 ACS on STN
- 131:74044 Synthesis of non-doped poly(3,4-ethylenedioxythiophene) and its spectroscopic data. Yamamoto, Takakazu; Abila, Mahmut (Research Laboratory of Resources Utilization, Tokyo Institute of Technology, Yokohama, Japan). Synthetic Metals, 100(2), 237-239 (English) 1999. CODEN: SYMEDZ. ISSN: 0379-6779. Publisher: Elsevier Science S.A..
- AB Non-doped poly(3,4-ethylenedioxythiophene) (PEDOT_h) has been synthesized by Ni-promoted dehalogenation polymn. of the corresponding 2,5-dichloro monomer. Its IR, NMR, and XRD data are compared with those of PEDOT_h prep'd. by chem. oxidn. polymn.
- IT **225518-49-0P**, 2,5-Dichloro-3,4-ethylenedioxythiophene
(prepn. and polycondensation of dichloroethylenedioxythiophene monomer)

RN 225518-49-0 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dichloro-2,3-dihydro- (9CI) (CA INDEX NAME)



IT **225518-50-3P**, 2,5-Dichloro-3,4-ethylenedioxythiophene homopolymer

(prepn. of undoped polymer by polycondensation)

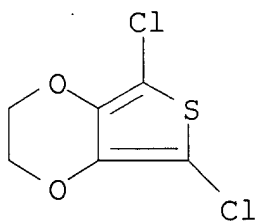
RN 225518-50-3 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,7-dichloro-2,3-dihydro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 225518-49-0

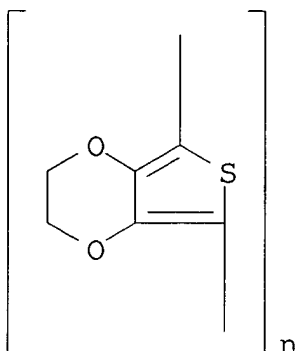
CMF C6 H4 Cl2 O2 S



IT **163359-60-2P**, Poly(3,4-ethylenedioxythiophene-2,5-diyl) (prepn. of undoped polymer by polycondensation of dichloro monomer)

RN 163359-60-2 HCA

CN Poly(2,3-dihydrothieno[3,4-b]-1,4-dioxin-5,7-diyl) (9CI) (CA INDEX NAME)



- IT Polymerization catalysts
(nickel complex; for polycondensation of dichloroethylenedioxythiophene monomer)
- IT 1295-35-8, Bis(1,5-cyclooctadiene)nickel
(catalyst for polycondensation of dichloroethylenedioxythiophene)
- IT 126213-50-1, 3,4-Ethylenedioxythiophene
(chlorination; prepn. of dichloroethylenedioxythiophene monomer)
- IT 111-78-4, 1,5-Cyclooctadiene 366-18-7, 2,2'-Bipyridyl
(in catalyst for polycondensation of dichloroethylenedioxythiophene)
- IT **225518-49-0P**, 2,5-Dichloro-3,4-ethylenedioxythiophene
(prepn. and polycondensation of dichloroethylenedioxythiophene monomer)
- IT **225518-50-3P**, 2,5-Dichloro-3,4-ethylenedioxythiophene homopolymer
(prepn. of undoped polymer by polycondensation)
- IT **163359-60-2P**, Poly(3,4-ethylenedioxythiophene-2,5-diyl)
(prepn. of undoped polymer by polycondensation of dichloro monomer)

L26 ANSWER 26 OF 29 HCA COPYRIGHT 2005 ACS on STN

124:203512 Absorption Properties of Alkoxy-Substituted

Thienylene-Vinylene Oligomers as a Function of the Doping Level. Havinga, E. E.; Mutsaers, C. M. J.; Jenneskens, L. W. (Philips Research Laboratories, Eindhoven, 5656 AA, Neth.). Chemistry of Materials, 8(3), 769-76 (English) 1996. CODEN: CMATEX. ISSN: 0897-4756. Publisher: American Chemical Society.

AB In an attempt to improve on the properties of PEDOT (poly(3,4-ethylenedioxythiophene)) as a stable, conducting, and transparent coating we synthesized four different alkoxy-substituted poly(thienylene-vinylene)s, 1-4, using the Stille coupling reaction. The oligomers and polymers obtained were characterized and their NIR-vis absorption spectra were measured as a function of doping, both electrochem. as films and chem. in soln. Similar spectra of

PEDOT films were gathered for comparison. In PEDOT a change in doping level does not change the energies of the absorption bands, while for the other polymers the bands shift markedly and the NIR peak at high doping level lies at a higher energy. The polymers 1-4 are much less suited for the intended coatings than PEDOT. Possible reasons for this are discussed.

IT 126213-54-5P 173291-56-0P

(absorption properties of alkoxy-substituted thienylene-vinylene oligomers as a function of the doping level)

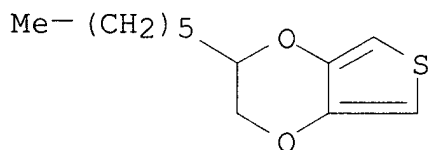
RN 126213-54-5 HCA

CN Thieno[3,4-b]-1,4-dioxin, 2-hexyl-2,3-dihydro-, homopolymer (9CI)
(CA INDEX NAME)

CM 1

CRN 126213-53-4

CMF C12 H18 O2 S



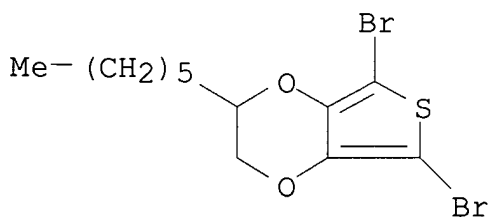
RN 173291-56-0 HCA

CN Stannane, 1,2-ethenediylbis[tributyl-, (E)-, polymer with
5,7-dibromo-2-hexyl-2,3-dihydrothieno[3,4-b]-1,4-dioxin (9CI) (CA
INDEX NAME)

CM 1

CRN 173291-50-4

CMF C12 H16 Br2 O2 S

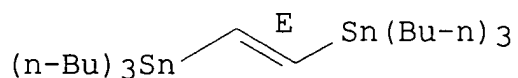


CM 2

CRN 14275-61-7

CMF C26 H56 Sn2

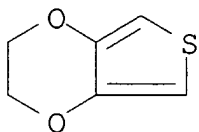
Double bond geometry as shown.



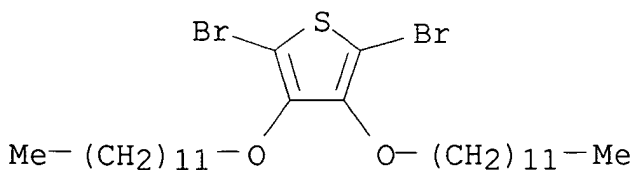
IT 126213-51-2, Poly(3,4-ethylenedioxythiophene)
 (absorption properties of alkoxy-substituted thienylene-vinylene
 oligomers as a function of the doping level)
 RN 126213-51-2 HCA
 CN Thieno[3,4-b]-1,4-dioxin, 2,3-dihydro-, homopolymer (9CI) (CA INDEX
 NAME)

CM 1

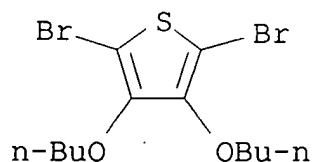
CRN 126213-50-1
 CMF C6 H6 O2 S



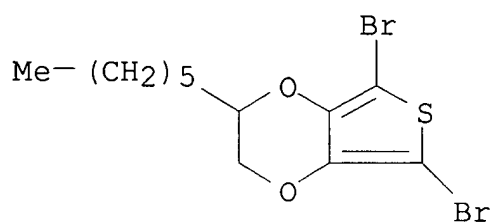
IT 173291-48-0P, 2,5-Dibromo-3,4-bis(dodecyloxy)thiophene
 173291-49-1P, 2,5-Dibromo-3,4-dibutoxythiophene
 173291-50-4P
 (monomer; absorption properties of alkoxy-substituted
 thienylene-vinylene oligomers as a function of the doping level)
 RN 173291-48-0 HCA
 CN Thiophene, 2,5-dibromo-3,4-bis(dodecyloxy)- (9CI) (CA INDEX NAME)



RN 173291-49-1 HCA
 CN Thiophene, 2,5-dibromo-3,4-dibutoxy- (9CI) (CA INDEX NAME)



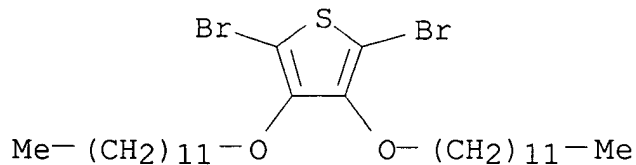
RN 173291-50-4 HCA
 CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2-hexyl-2,3-dihydro- (9CI)
 (CA INDEX NAME)



IT 173291-52-6P 173291-53-7P 173291-54-8P
 173291-55-9P
 (oligomeric; absorption properties of alkoxy-substituted
 thienylene-vinylene oligomers as a function of the doping level)
 RN 173291-52-6 HCA
 CN Stannane, 1,2-ethenediylbis[tributyl-, (E)-, polymer with
 2,5-dibromo-3,4-bis(dodecyloxy)thiophene (9CI) (CA INDEX NAME)

CM 1

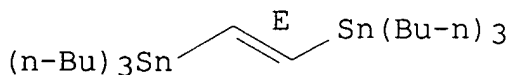
CRN 173291-48-0
 CMF C28 H50 Br2 O2 S



CM 2

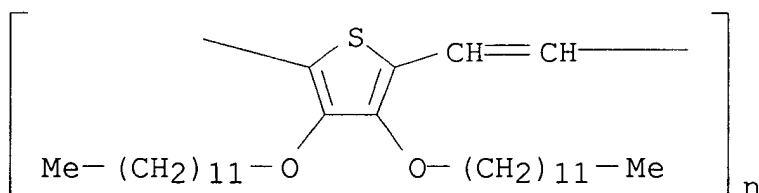
CRN 14275-61-7
 CMF C26 H56 Sn2

Double bond geometry as shown.



RN 173291-53-7 HCA

CN Poly[[3,4-bis(dodecyloxy)-2,5-thiophenediyl]-1,2-ethenediyl], (E)-
(9CI) (CA INDEX NAME)



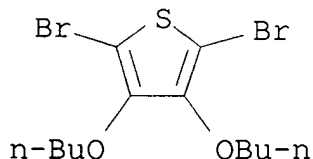
RN 173291-54-8 HCA

CN Stannane, 1,2-ethenediylbis[tributyl-, (E)-, polymer with
2,5-dibromo-3,4-dibutoxythiophene (9CI) (CA INDEX NAME)

CM 1

CRN 173291-49-1

CMF C12 H18 Br2 O2 S

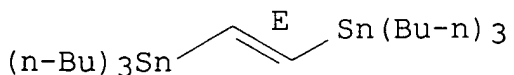


CM 2

CRN 14275-61-7

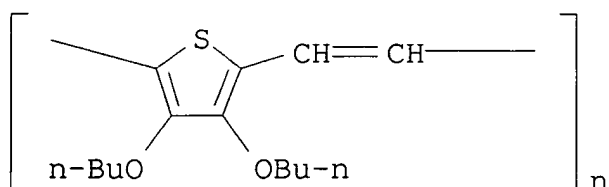
CMF C26 H56 Sn2

Double bond geometry as shown.



RN 173291-55-9 HCA

CN Poly[(3,4-dibutoxy-2,5-thiophenediyl)-1,2-ethenediyl], (E)- (9CI)
(CA INDEX NAME)



- IT Electric conductivity and conduction
 Electric conductors, polymeric
 Oscillator strength
 Ultraviolet and visible spectra
 (absorption properties of alkoxy-substituted thienylene-vinylene oligomers as a function of the doping level)
- IT Infrared spectra
 (near-; absorption properties of alkoxy-substituted thienylene-vinylene oligomers as a function of the doping level)
- IT Coating materials
 (elec. conductive, transparent, absorption properties of alkoxy-substituted thienylene-vinylene oligomers as a function of the doping level)
- IT Energy level, band structure
 (gap, absorption properties of alkoxy-substituted thienylene-vinylene oligomers as a function of the doping level)
- IT Electric potential
 (oxidn., absorption properties of alkoxy-substituted thienylene-vinylene oligomers as a function of the doping level)
- IT Polymers, properties
 (polythiophenes, -vinylenes; absorption properties of alkoxy-substituted thienylene-vinylene oligomers as a function of the doping level)
- IT **126213-54-5P 173291-56-0P 174592-79-1P**
 (absorption properties of alkoxy-substituted thienylene-vinylene oligomers as a function of the doping level)
- IT **126213-51-2, Poly(3,4-ethylenedioxythiophene)**
 (absorption properties of alkoxy-substituted thienylene-vinylene oligomers as a function of the doping level)
- IT 994-89-8P, Tributylethynyltin
 (absorption properties of alkoxy-substituted thienylene-vinylene oligomers as a function of the doping level)
- IT 84-58-2, 2,3-Dicyano-5,6-dichloro-1,4-benzoquinone 7705-08-0,
 Ferric chloride, reactions
 (dopant; absorption properties of alkoxy-substituted thienylene-vinylene oligomers as a function of the doping level)
- IT 128-08-5, N-Bromosuccinimide 120621-18-3, 3-(Dodecyloxy)thiophene
 (monomer synthesis; absorption properties of alkoxy-substituted thienylene-vinylene oligomers as a function of the doping level)

- IT 14275-61-7P, (E)-1,2-Bis(tributyltin)ethylene 173291-47-9P,
 2,5-Dibromo-3-(dodecyloxy)thiophene 173291-48-0P,
 2,5-Dibromo-3,4-bis(dodecyloxy)thiophene 173291-49-1P,
 2,5-Dibromo-3,4-dibutoxythiophene 173291-50-4P
 (monomer; absorption properties of alkoxy-substituted
 thienylene-vinylene oligomers as a function of the doping level)
- IT 173291-51-5P, (E)-1,2-Bis(tributyltin)ethylene-2,5-dibromo-3-
 (dodecyloxy)thiophene copolymer 173291-52-6P
 173291-53-7P 173291-54-8P 173291-55-9P
 174592-80-4P
 (oligomeric; absorption properties of alkoxy-substituted
 thienylene-vinylene oligomers as a function of the doping level)
- IT 14221-01-3, Tetrakis(triphenylphosphine)palladium(0)
 (polymn. catalyst; absorption properties of alkoxy-substituted
 thienylene-vinylene oligomers as a function of the doping level)
- IT 77214-82-5P
 (polymn. catalyst; absorption properties of alkoxy-substituted
 thienylene-vinylene oligomers as a function of the doping level)
- L26 ANSWER 27 OF 29 HCA COPYRIGHT 2005 ACS on STN
- 124:203135 Electrochromic Conducting Polymers via Electrochemical
 Polymerization of Bis(2-(3,4-ethylenedioxy)thienyl) Monomers.
 Sotzing, Gregory A.; Reynolds, John R.; Steel, Peter J. (Center for
 Macromolecular Science and Engineering, University of Florida,
 Gainesville, FL, 32611, USA). Chemistry of Materials, 8(4), 882-9
 (English) 1996. CODEN: CMATEX. ISSN: 0897-4756. Publisher:
 American Chemical Society.
- AB A series of bis(2-(3,4-ethylenedioxy)thiophene)-based monomers were
 synthesized and fully characterized; specifically
 (E)-1,2-bis(2-(3,4-ethylenedioxy)thienyl)vinylene (BEDOT-V),
 1,4-bis(2-(3,4-ethylenedioxy)thienyl)benzene (BEDOT-B),
 4,4'-bis(2-(3,4-ethylenedioxy)thienyl)biphenyl (BEDOT-BP),
 2,5-bis(2-(3,4-ethylenedioxy)thienyl)furan, 2,5-bis(2-(3,4-
 ethylenedioxy)thienyl)-thiophene (BEDOT-T), and 2,2':5',2''-ter(3,4-
 ethylenedioxy)thiophene, TER-EDOT. The X-ray crystal structures of
 BEDOT-V and BEDOT-B were detd. These monomers oxidize and
 polymerize at low potentials relative to other reported
 electropolymerizable heterocycles. The electroactive polymers
 formed have low redox switching potentials and are quite stable in
 the conducting state. TER-EDOT had the lowest peak oxidn. potential
 of +0.2 V vs Ag/Ag+, making it the most easily oxidized
 polymerizable thiophene monomer reported. The electronic band gaps
 of these EDOT based polymers were 1.4-2.3 eV (measured as the onset
 of the π - π^* transition) offering a diverse range of colors
 which may prove useful in electrochromic devices. For example,
 poly(BEDOT-V) is deep purple and opaque in the reduced state and
 transmissive sky blue in the oxidized state, poly(BEDOT-T) is deep
 blue opaque in the reduced state and transmissive blue in the

oxidized state, while poly(BEDOT-BP) is transmissive orange in the reduced state and opaque purple in the oxidized state. A thin film of poly(BEDOT-V) switched rapidly between redox states (under 2 s) with an initial optical contrast of 43%. This polymer retained 47% of its optical contrast and 48% of its original charge d. after 600 double potential steps.

IT 162899-00-5P 168641-47-2P 168641-48-3P

174508-35-1P 174508-36-2P 174508-37-3P

(electrochromic conducting polymers via electrochem. polymn. of bis(ethylenedioxy)thienyl) monomers)

RN 162899-00-5 HCA

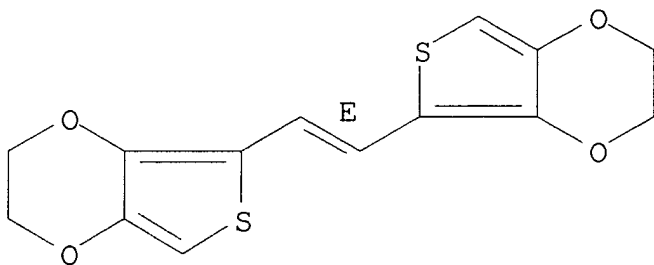
CN Thieno[3,4-b]-1,4-dioxin, 5,5'-(1,2-ethenediyl)bis[2,3-dihydro-, (E)-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 162898-99-9

CMF C14 H12 O4 S2

Double bond geometry as shown.



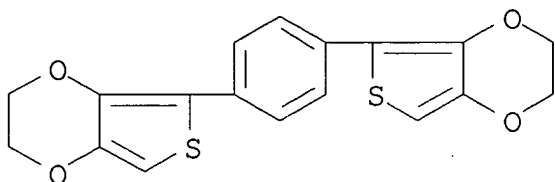
RN 168641-47-2 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,5'-(1,4-phenylene)bis[2,3-dihydro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 168641-43-8

CMF C18 H14 O4 S2



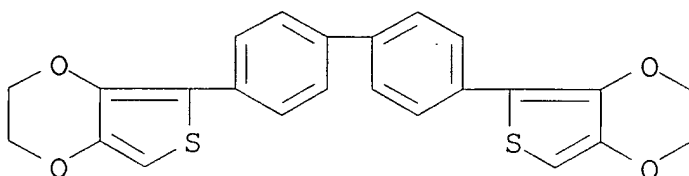
RN 168641-48-3 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,5'-([1,1'-biphenyl]-4,4'-diyl)bis[2,3-dihydro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 168641-44-9

CMF C24 H18 O4 S2



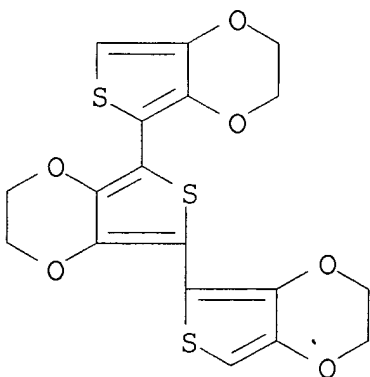
RN 174508-35-1 HCA

CN 5,5':7',5''-Terthieno[3,4-b]-1,4-dioxin, 2,2',2'',3,3',3''-hexahydro-
, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 174508-34-0

CMF C18 H14 O6 S3



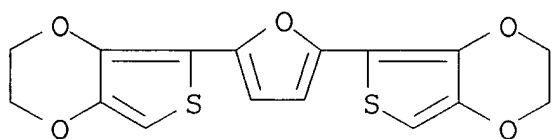
RN 174508-36-2 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,5'-(2,5-furandiyl)bis[2,3-dihydro-,
homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 174508-32-8

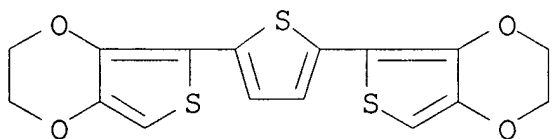
CMF C16 H12 O5 S2



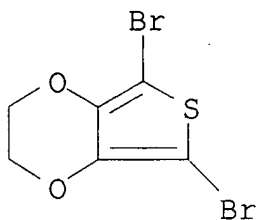
RN 174508-37-3 HCA
 CN Thieno[3,4-b]-1,4-dioxin, 5,5'-(2,5-thiophenediyl)bis[2,3-dihydro-,
 homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 174508-33-9
 CMF C16 H12 O4 S3

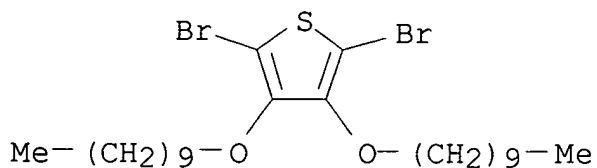


IT 174508-31-7P
 (intermediate; electrochromic conducting polymers via
 electrochem. polymn. of bis(ethylenedioxy)thienyl) monomers)
 RN 174508-31-7 HCA
 CN Thieno[3,4-b]-1,4-dioxin, 5,7-dibromo-2,3-dihydro- (9CI) (CA INDEX
 NAME)



IT Bond angle
 Bond length
 Crystal structure
 Electric conductors, polymeric
 (electrochromic conducting polymers via electrochem. polymn. of
 bis(ethylenedioxy)thienyl) monomers)
 IT Polymerization
 (electrochem., electrochromic conducting polymers via
 electrochem. polymn. of bis(ethylenedioxy)thienyl) monomers)
 IT Energy level, band structure

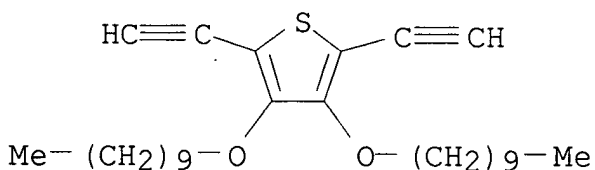
- (gap, electrochromic conducting polymers via electrochem. polymn. of bis(ethylenedioxy)thienyl) monomers)
- IT Polymers, preparation
(polythiophenes, electrochromic conducting polymers via electrochem. polymn. of bis(ethylenedioxy)thienyl) monomers)
- IT Crystallography
(x-ray, electrochromic conducting polymers via electrochem. polymn. of bis(ethylenedioxy)thienyl) monomers)
- IT 162899-00-5P 168641-47-2P 168641-48-3P
174508-35-1P 174508-36-2P 174508-37-3P
(electrochromic conducting polymers via electrochem. polymn. of bis(ethylenedioxy)thienyl) monomers)
- IT 32460-00-7P, 2,5-Dibromofuran. 162898-99-9P 168641-43-8P
174508-31-7P
(intermediate; electrochromic conducting polymers via electrochem. polymn. of bis(ethylenedioxy)thienyl) monomers)
- IT 168641-44-9P 174508-32-8P 174508-33-9P 174508-34-0P
(monomer; electrochromic conducting polymers via electrochem. polymn. of bis(ethylenedioxy)thienyl) monomers)
- IT 106-37-6, p-Dibromobenzene. 110-00-9, Furan 156-60-5
3141-27-3, 2,5-Dibromothiophene 126213-50-1, 3,4-Ethylenedioxythiophene
(starting material; electrochromic conducting polymers via electrochem. polymn. of bis(ethylenedioxy)thienyl) monomers)
- L26 ANSWER 28 OF 29 HCA COPYRIGHT 2005 ACS on STN
- 123:286791 The synthesis of decyloxy substituted poly(1,2-ethynediyl-2,5-thiophenediyls). McKellar, B. R.; Feld, William A. (Department Chemistry, Wright State University, Dayton, OH, 45435, USA). Polymer Preprints (American Chemical Society, Division of Polymer Chemistry), 35(2), 680-1 (English) 1994. CODEN: ACPPAY. ISSN: 0032-3934. Publisher: American Chemical Society, Division of Polymer Chemistry.
- AB An improved prepn. of 2,5-diethynyl-3,4-didecyloxythiophene (I) is reported. I was polymd. with 2,5-dibromo-3,4-didecyloxythiophene or 2,5-dibromothiophene to give polymers with thermal stability $\leq 200^\circ$.
- IT 169826-78-2P
(prepn. and polymn. of decyloxy-substituted thiophenes)
- RN 169826-78-2 HCA
- CN Thiophene, 3,4-bis(decyloxy)-2,5-diethynyl-, polymer with 2,5-dibromo-3,4-bis(decyloxy)thiophene (9CI) (CA INDEX NAME)
- CM 1
- CRN 169826-77-1
- CMF C24 H42 Br2 O2 S



CM 2

CRN 152189-52-1

CMF C28 H44 O2 S



IT 152189-52-1P

(prepn. and polymn. of decyloxy-substituted thiophene)

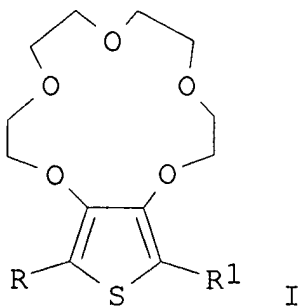
IT **169826-78-2P** 169826-79-3P

(prepn. and polymn. of decyloxy-substituted thiophenes)

L26 ANSWER 29 OF 29 HCA COPYRIGHT 2005 ACS on STN

122:315261 Synthesis and characterization of thiophenes, oligothiophenes and polythiophenes with crown ether units in direct π -conjugation. Baeuerle, P.; Scheib, St. (Inst. Organische Chemie, Universitaet Wuerzburg, Wuerzburg, D-97074, Germany). Acta Polymerica, 46(2), 124-9 (English) 1995. CODEN: ACPODY. ISSN: 0323-7648. Publisher: VCH.

GI



AB I (R,R' = 2-thiophenyl; R,R' = H; R = H, R' = 2-thiophenyl) were prepd. by substitution of I (R,R' = Br) with 2-(trimethylstannyl)thiophene, deacylation of I (R,R' = ethyloxycarbonyl), and substitution of I (R = H, R' = trimethylstannyl). I (R,R' = H; R = H, R' = 2-thiophenyl) were polymd. potentiodynamically to prep. selectively conducting polythiophenes with crown ether units in direct π -conjugation. The redox behavior of polymer films was characterized by cyclic voltammograms in MeCN solns. in the presence of Li⁺, Na⁺, and K⁺ cations, and by spectroelectrochem. measurements. The redox behavior of I (R,R' = H) polymer was effected by the introduction of cations, whereas that of I (R = H, R' = 2-thiophenyl) polymer was not. The sensitivity of I (R,R' = H) polymer to cations increased in the order: Na⁺ >> Li⁺ > K⁺.

IT 163657-78-1P 163657-79-2P

(prepn. and electrochem. properties of thiophenes and polythiophenes with crown ether units in direct π -conjugation)

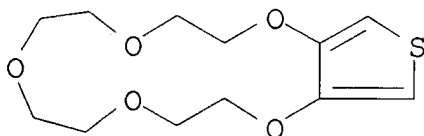
RN 163657-78-1 HCA

CN Thieno[3,4-b]-1,4,7,10,13-pentaoxacyclopentadecin,
2,3,5,6,8,9,11,12-octahydro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 122372-74-1

CMF C12 H18 O5 S



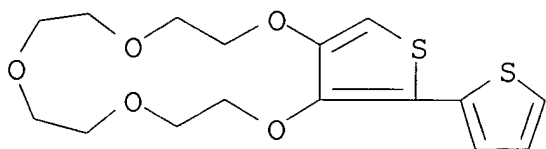
RN 163657-79-2 HCA

CN Thieno[3,4-b]-1,4,7,10,13-pentaoxacyclopentadecin,
2,3,5,6,8,9,11,12-octahydro-14-(2-thienyl)-, homopolymer (9CI) (CA
INDEX NAME) .

CM 1

CRN 163657-76-9

CMF C16 H20 O5 S2

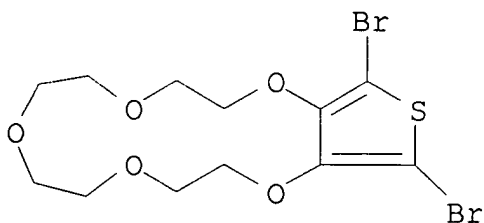


IT 163657-74-7P

(prepn. and electrochem. properties of thiophenes and polythiophenes with crown ether units in direct π -conjugation)

RN 163657-74-7 HCA

CN Thieno[3,4-b]-1,4,7,10,13-pentaoxacyclopentadecin, 14,16-dibromo-2,3,5,6,8,9,11,12-octahydro- (9CI) (CA INDEX NAME)



IT Electric conductors, polymeric
Electric current

(prepn. and electrochem. properties of thiophenes and polythiophenes with crown ether units in direct π -conjugation)

IT Polymerization

(electrochem., prepn. and electrochem. properties of thiophenes and polythiophenes with crown ether units in direct π -conjugation)

IT Electric potential

(oxidn., prepn. and electrochem. properties of thiophenes and polythiophenes with crown ether units in direct π -conjugation)

IT Polymers, preparation

(polythiophenes, crown ether group-contg., prepn. and electrochem. properties of thiophenes and polythiophenes with crown ether units in direct π -conjugation)

IT 3109-63-5, Tetrabutylammonium hexafluorophosphate 7601-89-0, Sodium perchlorate 7791-03-9, Lithium perchlorate 17084-13-8, Potassium hexafluorophosphate

(prepn. and electrochem. properties of thiophenes and polythiophenes with crown ether units in direct π -conjugation)

IT 163657-76-9P 163657-77-0P

(prepn. and electrochem. properties of thiophenes and polythiophenes with crown ether units in direct π -conjugation)

IT 163657-78-1P 163657-79-2P

- (prepn. and electrochem. properties of thiophenes and polythiophenes with crown ether units in direct π -conjugation)
- IT 1066-45-1, Trimethylstannyl chloride 3437-95-4, 2-Iodothiophene
37496-13-2, 2-(Trimethylstannyl)thiophene 122372-64-9
(prepn. and electrochem. properties of thiophenes and polythiophenes with crown ether units in direct π -conjugation)
- IT 163657-75-8P
(prepn. and electrochem. properties of thiophenes and polythiophenes with crown ether units in direct π -conjugation)
- IT 163657-74-7P
(prepn. and electrochem. properties of thiophenes and polythiophenes with crown ether units in direct π -conjugation)

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